

# Gaussian equivalent representation of functional integrals in quantum physics

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A new method is proposed for systematic approximate calculations of a large class of non-Gaussian functional integrals beyond the region of the perturbative expansion. This method provides a good accuracy of the lowest approximation, obtained in a simple way, which represents a generalization of the variational estimate if the functionals are real. In contrast to the variational approach, this method is applicable to complex functionals and theories with ultraviolet divergences. Higher-order corrections to the lowest approximation are evaluated by a regular scheme. This method is applied to different problems of theoretical physics: the polaron problem in solid-state physics, the phase-transition phenomenon in quantum field models, and the investigation of wave transmission in randomly distributed media. © 1995 American Institute of Physics.

## INTRODUCTION

In modern theoretical physics the formulation of quantum theory relying on the original classical system is mainly distinguished in two mutually complementary ways. One of them is the method of canonical quantization (CQ), where the field dynamical variables are considered as operators satisfying certain commutation relations and defined on a Hilbert space of states. Many papers have been devoted to CQ, and for the history and details we refer readers to Refs. 1 and 2.

The second formalism of quantization is Feynman's method of path integrals (PI).<sup>3,4</sup> The basic idea of the Feynman formulation of PI is that the quantum motion of a particle is considered as the sum of all quantum transitions along all possible classical trajectories with amplitudes proportional to

$$A[\mathbf{x}] \propto \exp\left(i \frac{S[\mathbf{x}]}{\hbar}\right),$$

where  $S[\mathbf{x}]$  is the classical action taken on a given trajectory  $\mathbf{x}$ . The total transition amplitude is assumed to be proportional to the integral

$$A \propto \int_{\Gamma} \delta\mathbf{r} \exp\left\{i \frac{1}{\hbar} S(t, \mathbf{x})\right\}, \quad (1)$$

where the classical action

$$S(t, \mathbf{r}) = \int_0^t d\tau \left\{ \frac{m^2}{2} \left| \dot{\mathbf{r}}(\tau) \right|^2 - V[\mathbf{r}(\tau)] \right\} \quad (2)$$

is taken along the given path  $\mathbf{r}(\tau)$ . The integration in (1) is performed over the space  $\Gamma$  of all possible "path-trajectories"  $\mathbf{r}(\tau)$  with  $0 < \tau < t_0$  for which  $\mathbf{r}(0) = \mathbf{x}_0$  and  $\mathbf{r}(t) = \mathbf{x}$ . This representation attracts much attention because it is close to the classical theory, having both physical clarity and

an elegant compact mathematical formulation. These advantages stimulated applications of PI to various problems in quantum physics.<sup>4</sup>

From a technical point of view, the PI formalism of quantization represents an essential attempt to go beyond the perturbation expansion and becomes effective for describing systems with infinite numbers of degrees of freedom.

In mathematics, Wiener<sup>5</sup> was the first to introduce, in 1920, the conception of PI to describe Brownian motion. Dirac first suggested a representation of a particle propagator in terms very close to PI techniques.<sup>6</sup> The systematic development of quantum mechanics (QM) within the PI approach is due to Feynman.

In quantum physics, Feynman<sup>3</sup> formulated nonrelativistic QM in the language of PI (in other words, functional or path integrals) and showed that this approach is completely equivalent to the solution of the Schrödinger equation. One of the main reasons for the popularity of "path integrals" is the understanding that classical mechanics becomes an approximation of QM in Feynman's formulation if one applies the method of "stationary phases" to the latter. In the classical limit  $\hbar \rightarrow 0$  the leading contribution to PI is given by the stationary points of the phase function  $S(t, \mathbf{r})$  in (1), which is the solution of Newton's classical equation of motion.

In 1949 Feynman used the functional integral (FI) for the construction of covariant QED (the Feynman diagrams).<sup>4</sup> After then, acknowledging the dignity of this new approach, Kac (1951) suggested a FI of Wiener's type for the representation of the evolution operator in Euclidean space.<sup>7</sup>

Path integration has come a long way since the 1950s. Probably the most famous early application of the FI in statistical physics was to the *polaron* (a nonrelativistic electron "dressed" by the surrounding quanta of lattice vibrations in ionic crystals). In polaron theory, the FI not only helps to formulate the answer qualitatively, but also remains the best way to calculate the answer more exactly than by other meth-

ods. It is a tractable field theory; the benefits obtained from using the FI are entirely analogous to those obtained in quantum field theory (QFT). But, in contrast to the polaron problem, all the steps for QFT are more difficult because of the divergences, the vector character of the fields, and gauge problems.

A number of investigators<sup>8,9</sup> independently came to the formulation of QFT in terms of the FI by considering variational estimates for Green functions.

A relatively simple way to represent the Green function of a quantized field within the FI was suggested in Ref. 10, where the equivalence of the FI over bosonic fields to the process of averaging over vacuum states of these fields was proved.

A new understanding of the FI was gained in Refs. 11 and 12, where the evolution operator of the model,  $P(\varphi)_2$ , in the Euclidean metric was represented in the FI form as

$$\exp\{-\beta H\} = \int d\sigma_0 \exp\left\{-\int dx P(\varphi)\right\}, \quad (3)$$

$$d\sigma_0 = C \delta\varphi \exp\left\{\frac{1}{2} \int dx [(\nabla\varphi)^2 + m^2\varphi^2]\right\},$$

where  $d\sigma_0$  is a Gaussian measure of integration, generated by the action  $S_0(\varphi) = 1/2 \int dx [(\nabla\varphi)^2 + m^2\varphi^2]$  of a free bosonic field and  $\int dx P(\varphi)$  introduced for a certain renormalization of the classical interaction  $\int dx P(\varphi)$ . This definition of the FI in (3), which allows the removal of interaction divergences coming from low-order "tadpole-type" diagrams, is the essentially new and important feature of the construction by Glimm and Jaffe.

The next important step in the application of the FI in QFT was taken in the quantization of Yang-Mills fields. A consistent scheme of quantization for a massless Yang-Mills field was constructed in 1967 by Faddeev and Popov<sup>13</sup> and by De Witt<sup>14</sup> within the PI approach. The FI turned out to be the shortest and most convenient method for constructing Feynman rules for perturbation expansions in gauge field theories. This method played an important role in the investigations of Slavnov,<sup>15</sup> Taylor,<sup>16</sup> Lee and Zinn-Justin,<sup>17</sup> and 't Hooft and Veltman.<sup>18</sup> In these papers a generalized Ward-Takahashi identity was obtained, various methods of invariant regularization were developed, and a procedure for renormalizing the perturbation series was given. Within the FI approach there has also been an attempt to construct a quantum theory of gravitation.<sup>19</sup>

In the 1970s, techniques based on the original ideas of Peak and Inomata<sup>20</sup> and of Duru and Kleinert<sup>21</sup> for solving certain non-Gaussian FIs occurring in QM have attracted much attention. Standard examples of QM considered in this approach are defined by using Bessel- and Legendre-type diffusion processes, other than the Wiener process often used in these subjects. These results do not require the machinery of stochastic analysis and can be treated in a quick, transparent way. A development of this method is assumed in Ref. 22, where certain non-Gaussian integrals with potentials like  $\sim 1/r^2$  or of the Morse type have been derived rigorously by using techniques of changing the dimension and time in FIs.

Excellent monographs and review papers have been devoted to the FI in quantum theory.<sup>13,23-29</sup>

Although many points concerning the correct mathematical definition and practical calculation of FIs still remain open, it is becoming clear that the description of a quantum system within the FI method is as convenient as the use of linear operators acting on vectors in Hilbert space within the method of CQ.

Nowadays, the FI method in quantum physics may be considered in two areas: (i) as a *convenient conception for qualitative consideration* of quantum theories<sup>30</sup> (e.g., gauge theories, renormalizable field models with fermions, etc.), which formulates the subject more clearly, with less formality in a mathematical sense, and more clearly because of the simplicity of using the quasiclassical (WKB) approximation, manifest relativistic covariance of the formulation, and ease in taking into account some specific constraints (e.g., the introduction of "ghosts" in the Yang-Mills theory); (ii) as a *practical tool for quantitative estimation* of characteristics of quantum systems (e.g., for models in QM and quantum statistics (QS),<sup>31</sup> supernormalizable scalar theories, solutions of differential equations, wave propagation in randomly distributed environments, etc.) because of the possibilities of reducing some dynamical variables by exact integration (e.g., in the polaron problem), changing space-time (for the inverse-square potential in QM), and convenience of computer calculations for the imaginary-time sum over paths,<sup>32</sup> etc.

In the present paper we consider mostly the second aspect of the application of FIs in quantum physics.

## 1. NONPERTURBATIVE METHODS FOR CALCULATING FUNCTIONAL INTEGRALS

A large number of problems of modern physics can be formulated in terms of the FI. Examples of such problems which will be considered in this paper are:

- investigation of the behavior of the polaron in ionic crystals in QS;
- phase transitions and phase restructuring in QFT models;
- propagation of waves in a stochastic medium with stochastically distributed centers.

All these problems have a common feature: their solution can be found in the form of a functional integral defined in the Gaussian measure, which by analogy with (3) can be written in the Euclidean region in the form

$$Z(g) = \int d\sigma_0 \exp\{gW[\varphi]\}, \quad (4)$$

where  $g$  is the coupling constant. Here, the functional measure

$$d\sigma_0 = C_0 \delta\varphi \exp\left\{-\frac{1}{2} (\varphi(x) D_0^{-1}(x,y) \varphi(y))\right\} \quad (5)$$

is of the Gaussian type and is defined by a Green function  $D_0$  corresponding to the differential operator  $D_0^{-1}(x,y)$ . As a rule, the normalization constant  $C_0$  is chosen in such way that  $\int d\sigma_0 \cdot 1 = 1$  or  $Z(0) = 1$ .



The interaction functional  $W[\varphi]$  usually provides the perturbation series  $Z(g) = \sum g^n Z_n$ , existing in any order  $n \geq 0$ .

Many important problems of quantum physics are related beyond perturbation theory. Their solution requires allowance for nonperturbative effects. There are many methods (analytical and computer simulation) for investigating these problems, but there is no generally accepted, universal technique.

Therefore, much effort has been devoted to the construction of methods for calculating these characteristics beyond the perturbative region. Nowadays the methods mainly used are: space-time transformations of path integrals, variational methods, the quasiclassical approximation (WKB), the  $1/N$  expansion, the instanton approximation, numerical methods with lattices, and so on. However, these methods have some limitations. For example, the WKB method cannot be used to study high-order quantum effects, and the  $1/N$  expansion gives poor convergence of the approximation series at real space-dimension numbers  $N=3$ . Direct numerical (lattice) simulation of these problems entails the difficulties of the continuous limit in lattice discretization and limited computer resources. Thus, the development of the FI method is continuing.

Usually, problems of this kind are studied by means of variational methods, which are popular because of their clear physical meaning and relatively simple calculations.

If the FI (4) is real, then variational methods can be used to estimate it. In the FI formulation, the principle of variational methods may be demonstrated following Feynman's simple example in QS. The partition function is written as

$$e^{-\beta F} = \int_{x(0)=x(\beta)} \delta x e^{-S[x]}, \quad (6)$$

where  $F$ ,  $\beta$ , and  $S$  are the free energy, the inverse temperature, and the action of the system, respectively. The integration is performed over paths  $x(u)$  defined on the interval  $u \in [0, \beta]$ . Suppose that we have another action,  $S_0$ , that is easier to work with. Then (6) can be rewritten as

$$e^{-\beta F} = \frac{\int \delta x e^{-S_0} e^{-(S-S_0)}}{\int \delta x e^{-S_0}} \cdot e^{-\beta F_0}, \quad (7)$$

where

$$e^{-\beta F_0} = \int \delta x e^{-S_0[x]}. \quad (8)$$

The first factor of (7) has the form of an average of  $e^{-(S-S_0)}$  with  $e^{-S_0}$  as the weight of a certain path  $x(u)$ . We can then write (7) as

$$e^{-\beta F} = \langle e^{-(S-S_0)} \rangle_{S_0} e^{-\beta F_0}. \quad (9)$$

Now we suppose that  $S$  and  $S_0$  are real and use Jensen's inequality

$$\langle e^{-f} \rangle \geq e^{-\langle f \rangle}. \quad (10)$$

Applying (10) to (9), we obtain

$$e^{-\beta F} \geq e^{-\langle S-S_0 \rangle} e^{-\beta F_0}, \quad (11)$$

where

$$\langle S-S_0 \rangle = \frac{\int \delta x (S-S_0) e^{-S_0}}{\int \delta x e^{-S_0}}. \quad (12)$$

Thus, we have a variational theorem:

$$F \leq F_0 + \frac{1}{\beta} \langle S-S_0 \rangle_{S_0}. \quad (13)$$

When a trial action  $S_0$  is introduced with some free parameters, which are then varied, we obtain a variational estimate of  $F$  in (13).

However, the variational technique does not provide a regular prescription for choosing the trial functional  $S_0$ , nor does it allow one to control the accuracy of the estimate. Moreover, there is a class of problems (most of the QFT models with ultraviolet (UV) divergences, complex and non-Hermitian functionals, and so on) to which the variational methods cannot be applied at all because the Jensen inequality no longer holds for these nonreal actions  $S$  and  $S_0$ .

## 2. GAUSSIAN EQUIVALENT REPRESENTATION OF FUNCTIONAL INTEGRALS

The main content of this section is the development of the method of *Gaussian equivalent representation (GER)* of FIs and its application to the investigation of the ground state (vacuum) of various QFT and QM models in order to study nonperturbative phenomena such as the strong-coupling regime, phase structure, and phase transitions.

The GER method is a type of generalization of the variational technique, but in contrast to the latter, it is efficient for QFT models with UV divergences and for theories with non-Hermitian and nonlocal actions (stochastic and dissipative processes), where variational methods cannot be used.

This method is characterized by a high accuracy of the lowest approximation, which can be obtained by simple and rapid calculations. It gives a regular prescription for the calculation of higher-order corrections to the lowest approximation and can be considered as the next step in the development of approximate-calculation methods.

### 2.1. General formalism

The study of many theoretical problems in statistical physics,<sup>33</sup> quantum field theory, and mathematical physics deals with a class of functional integrals defined on a Gaussian measure. We shall consider functional integrals of the general type (4) as follows:

$$\begin{aligned} Z_{\Gamma}(g) &= C_0 \int \delta \varphi \exp \left\{ -\frac{1}{2} (\varphi D_0^{-1} \varphi) + g W_0[\varphi] \right\} \\ &= \int d\sigma_0 \exp \{ g W_0[\varphi] \}. \end{aligned} \quad (14)$$

Here we have introduced the following notation for the Gaussian measure:

$$\begin{aligned} d\sigma_0 &= C_0 \delta \varphi \exp \left\{ -\frac{1}{2} (\varphi D_0^{-1} \varphi) \right\} \\ &= \frac{1}{\sqrt{\det D_0}} \prod_x d\varphi(x) \end{aligned} \quad (15)$$

$$\times \exp \left\{ -\frac{1}{2} \int_{\Gamma} \int_{\Gamma} dx dy \varphi(x) D_0^{-1}(x,y) \varphi(y) \right\}.$$

The Gaussian measure is normalized in such a way that  $\int d\sigma_0 \cdot 1 = 1$ . The integration in (14) is performed over functions  $\varphi(x)$  defined in a region  $\Gamma \subseteq R^d$  ( $d=1,2,\dots$ ). Usually, the region  $\Gamma$  is chosen as a multidimensional box:  $\Gamma = \{x: a_j \leq x_j \leq b_j, (j=1,\dots,d)\}$ .

A differential operator  $D_0^{-1}(x,y)$  is defined on functions  $\varphi(x)$  with appropriate boundary conditions. For example, the operator

$$D_0^{-1}(x,y) = \left( -\frac{\partial^2}{\partial x^2} + m_0^2 \right) \delta(x-y) \quad (16)$$

acts on functions satisfying certain periodic boundary conditions. The corresponding Green function  $D_0(x,y)$  satisfies the equation

$$\int_{\Gamma} dy D_0^{-1}(x,y) D_0(y,z) = \delta(x-z)$$

and ensures definite boundary conditions.

The parameter  $g$  is a coupling constant. The interaction functional  $W_0[\varphi]$  can be written in the general form

$$W_0[\varphi] = \int d\mu_a e^{i(a\varphi)}, \quad (17)$$

where we have introduced the notation

$$(a\varphi) = \int_{\Gamma} dy a(y) \varphi(y),$$

and  $d\mu_a$  is a functional measure. For example, for a potential having a Fourier transform one can write

$$W_0[\varphi] = \int_{\Gamma} dx U[\varphi(x)] = \int_{\Gamma} dx \int \frac{dk}{2\pi} \tilde{U}(k) \times \exp \left\{ i \int_{\Gamma} dy k \varphi(y) \delta(x-y) \right\}.$$

The FI in the representation (14) is well defined as a perturbation expansion in the coupling constant  $g$ . Thus, physically acceptable results can be obtained only in the weak-coupling regime  $g \ll 1$ . In this case the Gaussian measure  $d\sigma_0$  (15) gives the main contribution in the FI and corrections can be calculated by using a perturbation expansion.

The task is to give a representation of this integral in the strong-coupling regime.<sup>34</sup> Our idea is that the FI beyond the perturbation regime remains of the Gaussian type but with another Green function in the measure. In other words, we want to obtain a representation in which all the main contributions of the strong interaction are concentrated in the measure.

Let us perform the following transformations of the integral (14):

$$\begin{aligned} \varphi(x) &\rightarrow \varphi(x) + b(x), \\ D_0^{-1}(x,y) &\rightarrow D^{-1}(x,y), \end{aligned} \quad (18)$$

where  $b(x)$  is an arbitrary function and  $D(x,y)$  is an appropriate Green function of the differential operator  $D^{-1}$ ,

$$\int_{\Gamma} dy D^{-1}(x,y) D(y,z) = \delta(x-z),$$

providing the same boundary conditions.

The transformations (18) represent in a certain sense a functional analog of the standard canonical transformations made in the Hamiltonian formalism. The functional integral (14) takes the form

$$\begin{aligned} Z_{\Gamma}(g) &= \sqrt{\det \frac{D}{D_0}} \exp \left\{ -\frac{1}{2} (b D_0^{-1} b) \right\} \\ &\times \int d\sigma \exp \{ g W_1[\varphi, b, D] \}, \end{aligned} \quad (19)$$

where

$$\begin{aligned} d\sigma &= C \delta\varphi \exp \left\{ -\frac{1}{2} (\varphi D^{-1} \varphi) \right\}, \\ g W_1[\varphi, b, D] &= g W[\varphi + b] - (b D_0^{-1} \varphi) \\ &\quad - \frac{1}{2} (\varphi [D_0^{-1} - D^{-1}] \varphi), \end{aligned} \quad (20)$$

with the normalization condition  $\int d\sigma \cdot 1 = 1$ .

The tadpole Feynman diagrams give the main quantum contributions to the background energy of the system under consideration or, in other words, to the formation of the background state or vacuum. The mathematical problem is to take them into account correctly. In the quantum theory the main divergences given by tadpole vacuum diagrams are efficiently eliminated from consideration if the normal-ordered product of operators is introduced in the interaction Hamiltonian. Following this, the interaction functional in (19) must be written in the normal-ordered form. Thus, we must introduce in  $W_1$  the concept of the normal product according to the given Gaussian measure  $d\sigma$ . This can be done as follows:

$$:e^{i(a\varphi)}: = e^{i(a\varphi)} e^{1/2(aDa)}. \quad (21)$$

This definition leads to the relations

$$\int d\sigma :e^{i(a\varphi)}: = 1, \quad \int d\sigma : \varphi(x_1) \dots \varphi(x_n) : = 0.$$

After these transformations the functional in the integrand can be rewritten as

$$\begin{aligned} g W_1 &= g \int d\mu_a e^{i(ab) - 1/2(aDa)} :e_2^{i(a\varphi)}: \\ &+ \left[ g \int d\mu_a e^{i(ab) - 1/2(aDa)} - \frac{1}{2} ([D_0^{-1} - D^{-1}] D) \right] \\ &+ \left[ i g \int d\mu_a e^{i(ab) - 1/2(aDa)} (a\varphi) - (b D_0^{-1} \varphi) \right] \\ &- \frac{1}{2} \left[ g \int d\mu_a e^{i(ab) - 1/2(aDa)} (a\varphi)^2 \right. \\ &\quad \left. + (\varphi [D_0^{-1} - D^{-1}] \varphi) \right] :, \end{aligned} \quad (22)$$

where  $e_2^z = e^z - 1 - z - z^2/2$ .

Now we introduce the concept of the “correct form” of the action in the FI. We demand that the linear and quadratic terms in the integration variables  $\varphi(x)$  should be absent in the interaction functional  $W_I$  in (22). This requirement is argued in the same way. The system under consideration should be near its equilibrium point, so that any linear terms in the variable  $\varphi(x)$  must be absent. The quadratic configurations  $\sim \varphi^2$  determine the Gaussian oscillator character of the equilibrium point, and all of them are concentrated in the Gaussian measure  $d\sigma$  only. Therefore, they should not appear in the interaction functional, and

$$W_I \sim \varphi^3 \quad \text{for } \varphi \rightarrow 0.$$

Thus, the “correct form” requirement is satisfied if the following equations hold:

$$\begin{aligned} g \int d\mu_a i a(x) e^{i(ab) - 1/2(aDa)} - \int_{\Gamma} dy D_0^{-1}(x, y) b(y) &= 0, \\ g \int d\mu_a a(x) a(y) e^{i(ab) - 1/2(aDa)} + D_0^{-1}(x, y) \\ - D^{-1}(x, y) &= 0. \end{aligned} \quad (23)$$

These equations ensure the removal of the linear and quadratic terms from the interaction functional. Let us introduce the following functional and its correlation functions:

$$\begin{aligned} \hat{W}[b] &= \int d\mu_a \exp \left\{ i(ab) - \frac{1}{2}(aDa) \right\}, \\ w_n(x_1, \dots, x_n) &= \frac{\delta^n}{\delta b(x_1) \dots \delta b(x_n)} \hat{W}[b]. \end{aligned} \quad (24)$$

Equations (24) can be written in the form

$$\begin{aligned} b(x) &= g \int_{\Gamma} dy D_0(x, y) w_1(y), \\ D(x_1, x_2) &= D_0(x_1, x_2) \\ &+ g \int \int_{\Gamma} dy_1 dy_2 D_0(x_1, y_1) w_2(y_1, y_2) \\ &\times D(y_2, x_2). \end{aligned} \quad (25)$$

These equations determine the new Green function  $D(x_1, x_2)$  and the function  $b(x)$  in (22).

Finally, the new representation for the FI in (14) can be rewritten in the form

$$Z_{\Gamma}(g) = \exp\{E_0\} \cdot \int d\sigma \exp\{gW_I[\varphi]\}, \quad (26)$$

where

$$\begin{aligned} E_0 &= \frac{1}{2} \ln \det \left( \frac{D}{D_0} \right) - \frac{1}{2} (bD_0^{-1}b) - \frac{1}{2} ([D_0^{-1} - D^{-1}]D) \\ &+ g\hat{W}[b], \\ gW_I[\varphi] &= g \int d\mu_a e^{i(ab) - 1/2(aDa)} \cdot e_2^{i(a\varphi)} \dots \end{aligned} \quad (27)$$

The representation of the interaction functional in the normal-product form means that

$$\int d\sigma W_I[\varphi] = 0.$$

The function  $E_0$  defines the “energy” of the zeroth approximation. The next corrections to the leading term in (26) can be calculated by using a perturbation expansion over the new interaction functional  $W_I$ .

It should be stressed that the representations (14) and (26) are equivalent. Therefore the mathematical object  $Z_{\Gamma}(g)$  has at least two different representations (14) and (26). In principle other representations may exist if Eq. (26) has a more distinct solution. In this case we give preference to the representation in which the perturbation corrections connected with  $gW$  or  $gW_I$  are minimal for the given parameters.

All our transformations are valid for real and complex functions and functionals in the FI.

In the case of real FIs the representation (26) leads to following conclusion. Using Jensen’s inequality, one can get

$$Z_{\Gamma}(g) \geq \exp\{E_0\}, \quad (28)$$

so that  $E_0$  defines a lower bound for our FI.

On the other hand, one can easily check that (26) determines the minimum of the function  $E_0$ . Thus, the inequality (28) is the variational estimate of the initial FI. Moreover, the representation (26) makes it possible to calculate the perturbation corrections to  $E_0$  by developing the functional integral (26) over  $W_I$ .

## 2.2. The GER method for calculating the partition function

In this section we develop the main techniques of the GER method, especially for calculating the partition function in QM and QS. In other words, we deal with integrals where the field variable is the coordinate of a particle  $\mathbf{r}(t)$ , which is parametrized by the one-dimensional parameter  $t$ . For simplicity one can choose the symmetrical interval  $-T < t < T$ . The parameter  $T$  is connected with the time in QM or the inverse temperature  $2T = \beta$  in QS.

The partition function plays an important role in QS. For a large class of quantum-mechanical and quantum statistical problems describing the interaction of a quantum particle with a field or the propagation of waves and quantum particles through media with random or stochastic admixtures, the partition function can be represented in the form of a FI of the following general type:

$$\begin{aligned} Z_T(g) &= C_0 \int_{\mathbf{r}(-T)=\mathbf{r}(T)} d\mathbf{r} \exp \left\{ -\frac{1}{2} \int_{-T}^T dt \dot{\mathbf{r}}^2(t) \right. \\ &\left. + \frac{g}{2} \int \int_{-T}^T dt ds V(\mathbf{r}(t) - \mathbf{r}(s); t-s) \right\}. \end{aligned} \quad (29)$$

The standard normalization is  $Z_T(0) = 1$ . The integration in (29) is performed over all “paths” in a  $d$ -dimensional space satisfying periodic boundary conditions.

The kinetic term in the Gaussian measure can be written in the form

$$\int_{-T}^T dt \dot{\mathbf{r}}^2(t) = \int \int_{-T}^T dt ds \mathbf{r}(t) D_0^{-1}(t, s) \mathbf{r}(s),$$

$$D_0^{-1}(t, s) = -\frac{\partial^2}{\partial t^2} \delta(t-s). \quad (30)$$

The Green function  $D_0(t, s)$  corresponding to the differential operator  $D_0^{-1}(t, s)$  and satisfying the periodic boundary conditions is

$$D_0(t, s) = -\frac{1}{2} |t-s| - \frac{ts}{2T} \xrightarrow{T \rightarrow \infty} -\frac{1}{2} |t-s|. \quad (31)$$

The Fourier transform of this Green function is

$$\tilde{D}_0(p^2) = \int_{-\infty}^{\infty} dt e^{ipt} D_0(t)$$

$$= \frac{1}{2} \left[ \frac{1}{(p+i0)^2} + \frac{1}{(p-i0)^2} \right] \rightarrow \frac{1}{p^2}. \quad (32)$$

The parameter  $g$  is a coupling constant. In QM and QS, the potentials describing the influence of a field interaction or media on a quantum particle usually have a general form like  $V(\mathbf{r}-\mathbf{r}'; t-t')$ . Therefore we will consider this class of potentials further. The potential  $V(\mathbf{r}(t)-\mathbf{r}(s); t-s)$  in (29) is assumed to have the Fourier representation

$$V(\mathbf{r}(t)-\mathbf{r}(s); t-s) = \int \frac{d\mathbf{k}}{(2\pi)^d} \tilde{V}(\mathbf{k}; t-s) e^{i\mathbf{k}\mathbf{R}(t,s)}$$

$$= \int d\mathcal{H}(\mathbf{k}; t-s) e^{i\mathbf{k}\mathbf{R}(t,s)},$$

$$d\mathcal{H}(\mathbf{k}; t-s) = \frac{d\mathbf{k}}{(2\pi)^d} \tilde{V}(\mathbf{k}; t-s),$$

$$\mathbf{R}(t, s) = \mathbf{r}(t) - \mathbf{r}(s). \quad (33)$$

Thus, the initial FI in (29) can be rewritten as

$$Z_T(g) = \int d\sigma_0 \exp\{g W_0[\mathbf{r}]\}, \quad (34)$$

where

$$d\sigma_0 = C_0 d\mathbf{r} \exp\left\{-\frac{1}{2} \int \int_{-T}^T dt ds \mathbf{r}(t) D_0^{-1}(t, s) \mathbf{r}(s)\right\}, \quad (35)$$

$$g W_0[\mathbf{r}] = \frac{g}{2} \int \int_{-T}^T dt ds \int d\mathcal{H}(\mathbf{k}; t-s) e^{i\mathbf{k}\mathbf{R}(t,s)} \quad (36)$$

and the normalization condition is  $\int d\sigma_0 \cdot 1 = 1$ .

Now we are ready to apply the GER method to this FI. Note that for the potentials  $V(\mathbf{r}; t)$  of type (33) having their maximum at  $\mathbf{r}=0$  we do not need to introduce the function  $\mathbf{b}(t)$ , i.e.,  $\mathbf{b}(t)=0$ . According to the GER method, a new Gaussian measure should be introduced into the integral (34) as follows:

$$d\sigma = C d\mathbf{r} \exp\left\{-\frac{1}{2} \int \int_{-T}^T dt ds \mathbf{r}(t) D^{-1}(t-s) \mathbf{r}(s)\right\}. \quad (37)$$

The normalization constant  $C$  is  $\int d\sigma \cdot 1 = 1$ .

Second, we introduce the “normal-ordered” form of the potential (33) in the following way:

$$e^{i\mathbf{k}\mathbf{R}(t,s)} = :e^{i\mathbf{k}\mathbf{R}(t,s)}: \exp[-\mathbf{k}^2 F(t-s)], \quad (38)$$

where

$$F(t-s) = D(0) - D(t-s), \quad \int d\sigma R_i(t, s) R_j(t, s)$$

$$= 2 \delta_{ij} F(t-s).$$

In particular, the following relations are valid:

$$\int d\sigma :e^{i\mathbf{k}\mathbf{R}(t,s)}: = 1,$$

$$r_i(t) r_j(s) = :r_i(t) r_j(s): + \delta_{ij} D(t-s), \quad i, j = 1 \dots d.$$

The functional  $\hat{W}[b]$  in (24) becomes

$$\hat{W}[\mathbf{b}] = \frac{1}{2} \int \int_{-T}^T dt ds \int d\mathcal{H}(\mathbf{k}; t-s)$$

$$\times \exp[-\mathbf{k}^2 F(t-s)] e^{i\mathbf{k}(\mathbf{b}(t)-\mathbf{b}(s))}. \quad (39)$$

Its second correlation function is

$$\frac{\delta^2}{\delta b_i(t) \delta b_j(s)} \hat{W}[\mathbf{b}]|_{\mathbf{b}=0} = -\delta_{ij} \left[ \delta(t-s) \int_{-\infty}^{\infty} d\tau \Phi(\tau) \right.$$

$$\left. - \Phi(t-s) \right], \quad (40)$$

where

$$\Phi(\tau) = \frac{1}{d} \int d\mathcal{H}(\mathbf{k}; \tau) \mathbf{k}^2 \exp[-\mathbf{k}^2 F(\tau)].$$

Equation (26) defining the “correct form” of the interaction functional becomes

$$\tilde{\Sigma}(p^2) = \frac{1}{d} \int_{-\infty}^{\infty} d\tau [1 - \cos(p\tau)] \int d\mathcal{H}(\mathbf{k}; \tau) \mathbf{k}^2$$

$$\times \exp[-\mathbf{k}^2 F(\tau)], \quad (41)$$

$$F(\tau) = \int_0^{\infty} \frac{dp}{\pi} \frac{1 - \cos(p\tau)}{p^2 + g \tilde{\Sigma}(p^2)}. \quad (42)$$

Equations (41) and (42) define the Green function  $D(\tau)$ . For the asymptotic cases of weak ( $g \rightarrow 0$ ) and strong ( $g \rightarrow \infty$ ) interaction regimes, these equations may admit analytic solutions because one requires only that their behavior be within the accuracy of the first few leading-order terms such as  $\sim g, g^2$  or  $\sim 1/g, 1/g^2$ . In general, these are not solvable analytically, as they are nonlinear integral equations over functionals, but their solutions may be obtained by developing some numerical techniques. For example, the fixed-point method of successive iterations can be used. Starting from a trial function  $\tilde{\Sigma}_0(p^2)$ , we can calculate the iterations:

$$\tilde{\Sigma}_{n+1}(p^2) = \frac{1}{d} \int_{-\infty}^{\infty} d\tau [1 - \cos(p\tau)] \int d\mathcal{H}(\mathbf{k}; \tau) \mathbf{k}^2$$

$$\times \exp[-\mathbf{k}^2 F_n(\tau)],$$

$$F_{n+1}(\tau) = \int_0^\infty \frac{dp}{\pi} \cdot \frac{1 - \cos(p\tau)}{p^2 + g\tilde{\Sigma}_n(p^2)}. \quad (43)$$

This procedure can be developed for numerical solutions of (41) and (42). In this case, however, the initial trial functions  $F_0(\tau)$  and  $\tilde{\Sigma}_0(p^2)$  must be chosen reasonably, i.e., the iteration process (43) has to converge to solutions

$$\tilde{\Sigma}(p^2) = \tilde{\Sigma}_\infty(p^2) = \lim_{n \rightarrow \infty} \tilde{\Sigma}_n(p^2), \quad (44)$$

$$F(t) = F_\infty(t) = \lim_{n \rightarrow \infty} F_n(t). \quad (45)$$

For a reasonable choice of the trial functions, it is useful to investigate the asymptotic behavior of the solutions for Eqs. (41) and (42). An example of an analytic and a numerical solution of (41) and (42) is given in Sec. 3.3 for the polaron problem.

Substitution of (37)–(42) into (34) and the requirement that the new interaction functional be written in the “correct form” (see Sec. 2.1) lead to a new representation of the initial FI:

$$Z_T(g) = \exp(-2TE_0(g)) \cdot J_T(g), \quad (46)$$

$$J_T(g) = \int d\sigma \exp\{gW_I[\mathbf{r}]\},$$

where the interaction functional takes the form

$$gW_I[\mathbf{r}] = \frac{g}{2} \int \int_{-T}^T dt ds \int d\mathcal{R}(\mathbf{k}; t-s) \times \exp[-\mathbf{k}^2 F(t-s)] : e_2^{i\mathbf{k}\mathbf{R}(t,s)} :. \quad (47)$$

The function  $E_0(g)$ , being the “leading-order energy” or the energy in the zeroth approximation, is

$$E_0(g) = d \int_0^\infty \frac{dp}{2\pi} \left[ \ln \frac{\tilde{D}_0(p^2)}{\tilde{D}(p^2)} + p^2 \tilde{D}(p^2) - 1 \right] + \frac{g}{2} \int_{-\infty}^\infty d\tau \int d\mathcal{R}(\mathbf{k}; \tau) \exp[-\mathbf{k}^2 F(\tau)]. \quad (48)$$

Thus, the Gaussian equivalent representation of the initial FI in (34) is defined by (46)–(48). For a given potential  $V(\mathbf{r})$  we have a purely mathematical problem to solve [(41) and (42)] to find the Green function  $D(t, s)$ . Then we can compute the leading-order energy  $E(g)$  (48) and the highest corrections to it by perturbation calculations over the new interaction functional  $W_I$  (47).

### 3. THE POLARON PROBLEM

The polaron problem embraces a wide range of questions concerning the behavior of the conduction electron in polar crystals.<sup>35–37</sup> The first field-theoretical formulation of polaron theory was proposed by Fröhlich<sup>38</sup> to describe the interaction of a single band electron with phonons, the quanta associated with the longitudinal optical branch of lattice vibrations. Since that time, the Fröhlich polaron model has attracted interest as a testing ground of various nonper-

turbative methods in quantum physics. One of the main quasiparticle characteristics of the polaron is its ground-state energy (GSE)  $E_0(\alpha)$ .

Historically, the GSE of the polaron has been investigated in the weak,<sup>38</sup> intermediate,<sup>39</sup> and strong coupling regimes,<sup>40,41</sup> using different methods. The first attempt to construct a polaron theory, valid for arbitrary values of  $\alpha$ , was made by Feynman<sup>35</sup> within the path-integral (PI) formalism, using variational estimates. As a result, Feynman's PI approach gives good upper bounds on  $E_0(\alpha)$  in the entire range of  $\alpha$  in a unified way.

There arises the question of whether Feynman's estimates of the polaron GSE can be improved by introducing some trial actions more general than the quadratic action with two variational parameters used in Ref. 35. This question, in particular, has been studied in different variational approaches.<sup>42,43</sup> But in giving variational answers it could not estimate the next corrections to the values thus obtained.

Traditionally, the polaron problem has been investigated in three-dimensional ( $d=3$ ) space.<sup>44,45</sup> In recent years, however, polaron effects have been observed in low-dimensional systems,<sup>46</sup> and certain physical problems have been mapped into a two-dimensional ( $d=2$ ) polaron theory.<sup>47</sup> The possibility that an electron may be trapped on the surface of a dielectric material has attracted much interest.<sup>48</sup> The GSE of the polaron for  $d=2$  was discussed in Refs. 49 and 50.

In this section, we investigate the GSE of the polaron in the case of arbitrary space dimensions ( $d>1$ ) and try not only to improve Feynman's result, but also to estimate the next corrections that allow one to test the accuracy and reliability of the values thus obtained.

#### 3.1. Polaron path integral in $d$ dimensions

The Fröhlich longitudinal-optical (LO) polaron model for  $d=3$  is determined by the Hamiltonian

$$H = \frac{1}{2m} \mathbf{p}^2 + \hbar\omega \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} g_{\mathbf{k}} (a_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\mathbf{x}} - a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{x}}), \quad (49)$$

which describes the interaction of an electron (position and momentum vectors  $\mathbf{x}$  and  $\mathbf{p}$ , band mass  $m$ ) with the phonon field (creation and annihilation operators  $a_{\mathbf{k}}^\dagger$ ,  $a_{\mathbf{k}}$ , quantization volume  $\Omega$ , Planck constant  $\hbar$ ) associated with a LO branch of lattice vibrations (wave vector  $\mathbf{k}$  and frequency  $\omega$ ) in a polar crystal. The electron–phonon interaction coefficient for coupling with the wave vector  $\mathbf{k}$  in (49) is defined as follows:

$$g_{\mathbf{k}} = \frac{i\hbar\omega(\hbar/2m\omega)^{1/4}(4\pi\alpha)^{1/2}}{|\mathbf{k}|}, \quad (50)$$

where the dimensionless Fröhlich coupling constant  $\alpha$  takes the value  $\alpha \sim 1$ –20 in most of the real ionic crystals (e.g.,  $\alpha \approx 5$  for sodium chloride). In the following, units will be chosen such that  $\hbar = m = \omega = 1$ .

Until now, no nontrivial solution of the equation  $H\Psi_n = E_n\Psi_n$  was known. It has been shown<sup>51</sup> for generalized Fröhlich models that the function  $E_0(\alpha)$  has no points of nonanalyticity for arbitrary  $\alpha \geq 0$ . Various methods<sup>35,39,40,52</sup>



have been used to calculate approximately the spectrum of  $H$ , especially to obtain its GSE  $E_0$  for selected (weak, intermediate, or strong) regions of  $\alpha$ .

To extend the Fröhlich Hamiltonian (49) written for  $d=3$  to arbitrary spatial dimensions  $d>1$ , we follow a physical approach<sup>53,54</sup> inspired by the formulation of a lower-dimensional polaron problem obtained from the Fröhlich Hamiltonian of a higher-dimensional system by integrating out one or more dimensions. Following Ref. 54, we assume that the form of the Fröhlich Hamiltonian in  $d$  dimensions is the same as in (49), except that now all the vectors and operators are  $d$ -dimensional, and the electron-phonon interaction coefficient  $g_{\mathbf{k}}$  is redefined as follows:

$$|g_{\mathbf{k}}|^2 = \frac{\lambda_d^2}{|\mathbf{k}|^{d-1}}, \quad \lambda_d^2 = \Gamma\left(\frac{d-1}{2}\right) 2^{d-3/2} \pi^{(d-1)/2} \alpha. \quad (51)$$

Accordingly, we write the FI representation of the free energy  $F(\beta)$  of a polaron with a given temperature  $\Theta=1/\beta$  as follows:

$$\exp(-\beta F) = \text{Tr}[\exp(-\beta H)], \quad (52)$$

where the Hamiltonian  $H$  in (49) must be written in terms of the coordinates and momenta. The "trace"  $\text{Tr}=\text{Tr}_{\text{el}}\text{Tr}_{\text{ph}}$  here is assumed to be taken over the whole space of states of the "electron+phonon" system.

It is well known from the famous paper by Feynman<sup>35</sup> that the path-integral approach to the polaron has an advantage because the phonon trace  $\text{Tr}_{\text{ph}}$  in (52) can be adequately eliminated and, as a consequence, the polaron problem is reduced to an effective one-particle problem with a retarded interaction. The result reads

$$Z_{\beta}(\alpha) = \exp(-\beta F) = \int_{\mathbf{x}(0)=\mathbf{x}(\beta)} \delta \mathbf{x} \exp(S[\mathbf{x}]), \quad (53)$$

where the action  $S[\mathbf{x}]$  is

$$S[\mathbf{x}] = -\frac{1}{2} \int_0^{\beta} dt \dot{\mathbf{x}}^2(t) + \frac{\lambda_d^2}{8\pi} \int \int_0^{\beta} dt ds \frac{1}{|\mathbf{x}(t) - \mathbf{x}(s)|} \frac{e^{|t-s|} + e^{\beta-|t-s|}}{e^{\beta} - 1}. \quad (54)$$

The free energy  $F(\beta)$  tends to the GSE as  $\beta \rightarrow \infty$  (zero-temperature case):

$$E_0 = -\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln Z_{\beta}(\alpha). \quad (55)$$

The path integral in (53) is not explicitly solvable, owing to the non-Gaussian character of  $S$ . For its variational estimation for  $d=3$ , Feynman proposed<sup>35</sup> a quadratic two-body trial action  $S_F$  instead of  $S$ :

$$S[\mathbf{x}] \rightarrow S_F[\mathbf{x}] = -\frac{1}{2} \int_0^{\beta} dt \dot{\mathbf{x}}^2(t) + \frac{C}{2} \int \int_0^{\beta} dt ds [\mathbf{x}(t) - \mathbf{x}(s)]^2 \exp\{-w|t-s|\}, \quad (56)$$

where the constants  $C$  and  $w$  are variational parameters. With the trial action  $S_F$  one gets an exact solution for the

path integral in (53). A variation for finding the absolute minimum of  $E_0^F(\alpha) = F_F(\alpha)$  for  $\beta \rightarrow \infty$  in the parameters  $C$  and  $w$  leads to a rigorous upper bound on the polaron GSE at arbitrary  $\alpha$ , which is Feynman's well known result.<sup>35</sup>

Here we will show that the application of the GER method improves Feynman's estimate. We consider the polaron GSE in the case of arbitrary space dimension  $d>1$  and start again from the FI in (53) and (54).

For further convenience, to get a symmetrical region over  $t$ ,<sup>56</sup> and we change the variable of the FI in (53) to

$$\mathbf{x}(t) \rightarrow \mathbf{r}(t-T), \quad T = \beta/2, \quad (57)$$

with the electron motion  $\mathbf{r}(t)$  embedded in  $d$ -dimensional space. Accordingly, the GSE of the Fröhlich polaron  $E_0(\alpha)$  [it will hereafter be denoted by  $E(\alpha)$ ] can be determined as follows:

$$E(\alpha) = -\lim_{T \rightarrow \infty} \frac{1}{2T} \ln Z_T(\alpha), \quad (58)$$

where a FI is introduced<sup>55</sup> in the form

$$Z_T(\alpha) = C_0 \int_{\mathbf{r}(-T)=\mathbf{r}(T)} \delta \mathbf{r} \exp \left\{ -\frac{1}{2} (\mathbf{r} D_0^{-1} \mathbf{r}) + \frac{\alpha}{2} \int \int_{-T}^T dt ds V[\mathbf{r}(t) - \mathbf{r}(s); t-s] \right\},$$

$$C_0 = \sqrt{\det D_0^{-1}}, \quad (\mathbf{r}, D_0^{-1} \mathbf{r}) = \int \int_{-T}^T dt ds \mathbf{r}(t) D_0^{-1}(t,s) \mathbf{r}(s). \quad (59)$$

The standard normalization  $E(0)=0$  in (58) is satisfied under the condition  $Z_T(0)=1$ .

The free-electron system is described by the kinetic term  $(\mathbf{r} D_0^{-1} \mathbf{r})$ , where the differential operator  $D_0^{-1}$  and its Green function  $D_0$  are given by (30) and (31) in the previous section for  $T \rightarrow \infty$ .

The Coulomb-like interaction part, the electron self-interaction, is given by the retarded potential

$$V[\mathbf{R}; t-s] = \frac{\Gamma(d/2-1/2)}{4\sqrt{2}\pi^{(d+1)/2}} e^{-|t-s|} \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}} \exp(i\mathbf{k}\mathbf{R}), \quad (60)$$

with the electron position vector  $\mathbf{r}(t)$  embedded into  $d$  dimensions.

The path integral in (59) is not explicitly solvable, owing to the non-Gaussian character of  $V[\mathbf{R}; t-s]$  in (60).

### 3.2. Bounds for the polaron ground-state energy in $d$ dimensions

??? For  $\alpha$  not too large, the PI in the initial representation (59) can be estimated by using a perturbation expansion in  $\alpha$ . The problem is to estimate  $Z_T(\alpha)$  beyond the weak-coupling regime. Accordingly, we can apply the GER method to this problem.

Our key steps will be the same as those in the previous section. We recall that these are:

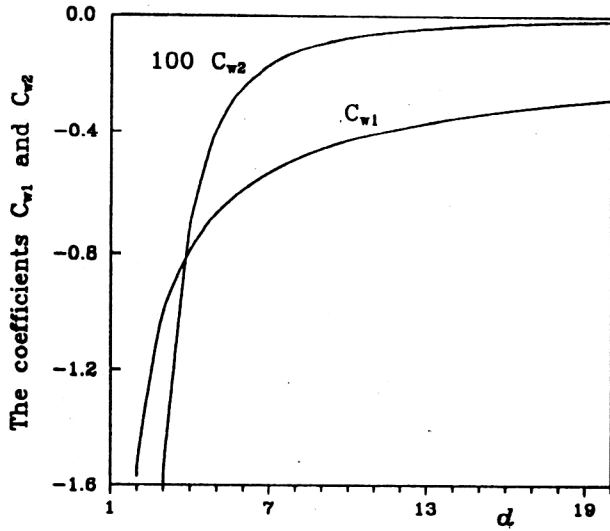


FIG. 1. Behavior of the coefficients  $C_{w1}$  and  $C_{w2}$  of the polaron ground-state energy  $E(\alpha) = \alpha \cdot C_{w1} + \alpha^2 \cdot C_{w2} + O(\alpha^3)$  in the weak-coupling limit  $\alpha \rightarrow 0$ , in its dependence on the number of space dimensions  $d$ .

(i) the introduction of a new Gaussian measure  $d\sigma$  (20) standing for the kinetic part of the FI, which forms a new representation of the initial FI;

(ii) the requirements of the “normal-ordered” and “correct” form of the interaction part of the FI in this representation, which is reached by introducing the constraint equations (41) and (42).

This scheme results in a new representation of the initial FI: an exponential with the leading term of energy factored out as a free multiplicand (48), and all the corrections to it defined by another FI (47).

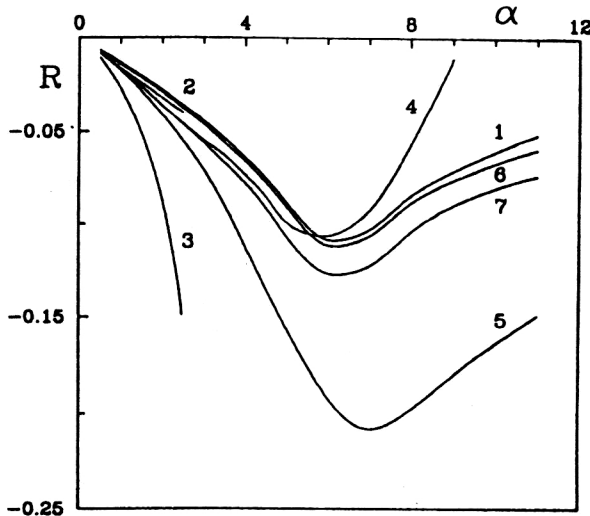


FIG. 2. Some known results for the polaron ground-state energy  $E$  (in three-dimensional space), displayed as a function of the electron-phonon coupling constant  $\alpha$ . For clarity, the ratio  $R = (E_* - E_{\text{harm}}) / |E_{\text{harm}}|$  is shown, where  $E_*$  are estimates obtained in Refs. 52, 86, 89, and 97, and  $E_{\text{harm}}$  is the “harmonic-oscillator” approximation.<sup>86</sup> In these units the curve for  $E_{\text{harm}}$  coincides with the abscissa axis. The curves correspond to the estimates: 1—Feynman’s upper; 2/3—Larsen’s upper/lower; 4/5—Smondyrev’s upper/lower; 6—our  $E_0(\alpha)$ ; 7—our  $E^{(2)}(\alpha)$ .

Performing the operations of this scheme and using Eqs. (41), (42), and (46)–(48), we obtain the new representation (47) of the GSE of the optical polaron in the GER method as follows:

$$E(\alpha) = E_0(\alpha) + \Delta E(\alpha), \quad (61)$$

where the function  $E_0(\alpha)$ , being the “leading-order energy” or the GSE in the zeroth approximation, is [see Eq. (48)]

$$E_0(\alpha) = -d \left\{ \frac{1}{2\pi} \int_0^\infty dk [\ln(k^2 \tilde{D}(k)) - k^2 \tilde{D}(k) + 1] + \frac{\alpha_d}{3\sqrt{2\pi}} \int_0^\infty dt \frac{\exp(-t)}{F^{1/2}(t)} \right\}. \quad (62)$$

The function  $F(t)$  in (62) is defined by the equations [see Eqs. (41) and (42)]

$$F(t) = \int_{-\infty}^\infty \frac{dk}{2\pi} \tilde{D}(k) (1 - e^{ikt}) = \frac{1}{\pi} \int_0^\infty dk \frac{1 - \cos(kt)}{k^2 + \alpha_d \tilde{\Sigma}(k)}, \quad (63)$$

$$\tilde{\Sigma}(k) = \int_{-\infty}^\infty dt e^{-ikt} \Sigma(t) = \frac{1}{3\sqrt{2\pi}} \int_0^\infty dt \times \exp(-t) \frac{1 - \cos(kt)}{F^{3/2}(t)}. \quad (64)$$

Here we have introduced the “effective coupling constant”

$$\alpha_d = \alpha \cdot R_d, \quad R_d = \frac{3\sqrt{\pi}\Gamma(d/2 - 1/2)}{2d\Gamma(d/2)}. \quad (65)$$

Our leading term (the zeroth-order approximation)  $E_0(\alpha)$  gives an upper bound on the exact GSE of a polaron  $E(\alpha)$ . Actually, applying Jensen’s inequality to (61), we obtain

$$\exp\{-2T \cdot E(\alpha)\} \geq \exp\{-2T \cdot E_0(\alpha)\}. \quad (66)$$

Consequently,

$$E_0(\alpha) \geq E(\alpha). \quad (67)$$

The high-order corrections  $\Delta E(\alpha)$  in (61) can be obtained by evaluating the PI

$$\exp\{-2T \cdot \Delta E(\alpha)\} = C \int_{\mathbf{r}(-T)=\mathbf{r}(T)} \delta \mathbf{r} \times \exp \left\{ -\frac{1}{2} \int_{-T}^T \int_{-T}^T dt ds \mathbf{r}(t) D^{-1} \times (t, s) \mathbf{r}(s) + W[\mathbf{r}] \right\}. \quad (68)$$

Here, the interaction functional written in the new representation is

$$W[\mathbf{r}] = \alpha_d \cdot \frac{\Gamma(d/2)d}{6\sqrt{2\pi}d^{2+1}} \int_{-T}^T \int_{-T}^T dt ds e^{-|t-s|} \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}} \times \exp\{-\mathbf{k}^2 F(t-s)\} : e^{i\mathbf{k} \cdot (\mathbf{r}(t) - \mathbf{r}(s))} :, \quad (69)$$

where  $e_x^x = e^x - 1 - x - x^2/2$ .

Owing to (64) and (63) in the new representation, all the quadratic terms in the polaron action functional are concentrated only in the new Gaussian measure  $d\sigma$  and do not enter into  $W[\mathbf{r}]$ .

It should be stressed that the representation (61) is completely equivalent to the initial representation (58) for asymptotically large  $T \rightarrow \infty$ . The Gaussian equivalent representation (61) gives the origin of various approximations differing from each other in the accuracy of deriving Eqs. (63) and (64).

As a simple approximation to  $\tilde{\Sigma}(k)$  obeying the necessary asymptotic conditions, one can take the function

$$\tilde{\Sigma}(k) = \frac{\mu^2}{\alpha_d} \cdot \frac{k^2}{\xi^2 + k^2}, \quad (70)$$

where  $\mu$  and  $\xi$  are parameters. Then (62) becomes

$$E_0(\alpha) = -\frac{d}{2} \left[ \xi - \lambda + \frac{\mu^2}{2\lambda} \right] - \frac{\alpha_d \lambda^{3/2} d}{3\mu\sqrt{\pi}} \int_0^\infty \frac{dt \exp(-t)}{\sqrt{1 - \exp(-\lambda t) + \lambda t \xi^2/\mu^2}},$$

$$\lambda = \sqrt{\mu^2 + \xi^2}. \quad (71)$$

Minimizing this energy in the parameters  $\mu$  and  $\xi$ , one easily finds a variational upper bound in  $d$  dimensions. For  $d=3$  ( $\alpha_3 = \alpha$ ) it explicitly reproduces the well-known Feynman variational upper bound on the polaron GSE:<sup>35</sup>

$$E^{\text{Feynman}}(\alpha) = \min_{\mu} \min_{\xi} E_0(\alpha, d=3). \quad (72)$$

We stress that the extremal conditions on the parameters  $\mu$  and  $\xi$  in (72) are equivalent to a particular choice of the functions  $\tilde{\Sigma}(k)$  in (70). However, the function in (70) is not an exact solution of (63) and (64). This means that Feynman's trial quadratic action does not represent entirely the Gaussian part of the polaron action for  $d=3$ . Exact numerical solution of Eqs. (63) and (64) by the iteration procedure allows us to obtain  $E_0(\alpha)$  more exactly, which improves Feynman's result  $E^F(\alpha)$  in the entire range of  $\alpha$ . The numerical results  $E_0(\alpha)$  for  $d=2$  and  $d=3$ , as compared with Feynman's variational estimation, are displayed in Tables I–VI.

The correction  $\Delta E(\alpha)$  must be evaluated from the functional integral in (69) by expanding  $e^W$  in (68) in a series:

$$\Delta E(\alpha) = \sum_{n=1}^{\infty} \Delta E_n(\alpha) = -\lim_{T \rightarrow \infty} \frac{1}{2T} \sum_{n=1}^{\infty} \frac{1}{n!} \int d\sigma \{W[\mathbf{r}]\}_{\text{connected}}^n. \quad (73)$$

We stress that (73) is not a standard perturbation series in the coupling constant  $\alpha_d$ , as  $\alpha_d$  enters into  $W$  not only explicitly as a factor, but also implicitly through the function  $F(t)$ . The first term in (73) with  $n=1$  is equal to zero, owing to the

normal ordering. Nontrivial corrections are given by the terms with  $n \geq 2$ . For the second-order correction to  $E_0(\alpha)$  we get

$$\Delta E_2(\alpha) = -\alpha_d^2 \cdot \frac{\Gamma(d/2)d^2}{18\pi^{3/2}} \sum_{n=2}^{\infty} Q_n R_n(\alpha), \quad (74)$$

where

$$Q_n = \frac{(2n)! \Gamma(n+1/2)}{16^n (n!)^2 \Gamma(n+d/2)},$$

$$R_n = \int \int_0^\infty \int d a d b d c \left\{ e^{-a-c} \times \frac{[F(a+b) + F(b+c) - F(a+b+c) - F(b)]^{2n}}{[F(a) \cdot F(c)]^{n+1/2}} + e^{-a-2b-c} \times \frac{[F(a) + F(c) - F(a+b+c) - F(b)]^{2n}}{[F(a+b) \cdot F(b+c)]^{n+1/2}} + e^{-a-2b-c} \times \frac{[F(a+b) + F(b+c) - F(a) - F(c)]^{2n}}{[F(a+b+c) \cdot F(b)]^{n+1/2}} \right\}.$$

We stress that the expression (74) can be further simplified, but we keep this form for clarity.

Finally, we get the following expression for the GSE of the polaron:

$$E^{(2)}(\alpha) = E_0(\alpha) + \Delta E_2(\alpha), \quad (75)$$

which can be evaluated numerically for arbitrary  $\alpha$  and different space dimensions  $d$ .

Notice that  $E_0(\alpha)$  in (62) is of order  $\alpha^i$  ( $i=0,1,2,\dots$ ), while  $\Delta E_2(\alpha)$  in (74) is only of order  $\alpha^j$  ( $j=2,3,\dots$ ).

The theory under consideration has two parameters  $\alpha$  and  $d$ . In general, all our expressions should depend on both of them. Notice that the key expressions in (63) and (64), completely defining the functions  $F(t)$  and  $\tilde{\Sigma}(k)$ , depend only on the effective coupling constant  $\alpha_d$ . This means that the relations

$$F^{[n]}(\alpha_m, t) = F^{[m]}(\alpha_n, t), \quad \tilde{\Sigma}^{[n]}(\alpha_m, k) = \tilde{\Sigma}^{[m]}(\alpha_n, k),$$

$$n, m > 1, \quad (76)$$

hold, where the numbers of space dimensions  $n$  and  $m$  are in square brackets [...]. In the particular case of  $d=2$  and  $d=3$ , we found

$$F^{[2]}(\alpha, t) = F^{[3]} \left( \frac{3\pi\alpha}{4}, t \right), \quad \tilde{\Sigma}^{[2]}(\alpha, k) = \tilde{\Sigma}^{[3]} \left( \frac{3\pi\alpha}{4}, k \right). \quad (77)$$

Then, considering (62), one easily finds that this scaling relation is also valid for  $(1/d)E_0(\alpha_d)$ . We have

$$E_0^{[2]}(\alpha) = \frac{2}{3} E_0^{[3]} \left( \frac{3\pi\alpha}{4} \right). \quad (78)$$

Note that the relation (78) was obtained earlier in Refs. 50 and 54. But this scaling is not valid beyond  $E_0$  because the interaction functional  $W[\mathbf{r}]$  depends not only on  $\alpha_d$ , but also on  $d$  in a complicated way.

Let us consider the asymptotic limits of spatial dimensions  $d$  at fixed finite  $\alpha$ . We get

$$\lim_{d \rightarrow 1} \alpha_d = \frac{3\alpha}{d-1} \rightarrow \infty, \quad \lim_{d \rightarrow \infty} \alpha_d = \frac{3\alpha\sqrt{\pi e}}{\sqrt{2}d^{3/2}} \rightarrow 0. \quad (79)$$

Taking into account (79), we can conclude that as  $d$  becomes larger,  $\alpha_d$  decreases rapidly and in fact we are dealing with the effective weak-coupling regime  $\alpha_d \ll 1$  even for  $\alpha$  not too small. For example, the second-order corrections  $\Delta E_2(\alpha)$  behave as follows:

$$\Delta E_2(\alpha) \xrightarrow{d \rightarrow \infty} -\frac{1}{8\pi} \alpha_d^2 \rightarrow 0. \quad (80)$$

In other words, our leading-order energy term  $E_0(\alpha)$  tends to the exact GSE  $E(\alpha)$  as  $d$  grows because the role of  $\Delta E(\alpha)$  becomes insignificant.

### 3.3. Numerical results

In this section, we present numerical values of  $E_0(\alpha)$  and  $E^{(2)}(\alpha)$ , estimated by the GER method, and compare them with known results obtained in various (weak, strong, and intermediate) ranges of  $\alpha$ . The results are given in Tables I–VI.

#### A. Weak-coupling limit

Among the known numerical results concerning the GSE of the polaron, the more accurate ones are those obtained for  $\alpha \rightarrow 0$ . Below, we calculate the exact GSE of the  $d$ -dimensional polaron for the order  $\alpha^2$  in the weak-coupling limit and compare the accuracy of the results with exact perturbation estimates presented in Refs. 49, 52, 54, and 58–60 for  $d=2$  and  $d=3$ .

For  $\alpha$  not too large, the polaron self-energy  $E(\alpha)$  has the form

$$E(\alpha) = \alpha \cdot C_{w1} + \alpha^2 \cdot C_{w2} + O(\alpha^3). \quad (81)$$

The coefficients  $C_{w1}$  and  $C_{w2}$  are known with good accuracy for  $d=2$  (Ref. 54) and  $d=3$  (Refs. 54 and 58). In our approach, the coefficient  $C_{w1}$  arises only from  $E_0(\alpha)$  in (62), whereas the  $C_{w2}$  come from both  $E_0(\alpha)$  and  $\Delta E_2(\alpha)$  in (74). We get the coefficients  $C_{w1}$  and  $C_{w2}$  exactly as follows:

$$C_{w1} = -\frac{R_d}{3} d \quad (82)$$

TABLE I. Comparison of known weak-coupling results for the polaron ground-state energy  $E(\alpha) = \alpha \cdot C_{w1} + \alpha^2 \cdot C_{w2} + O(\alpha^3)$  in two dimensions.

| Authors                                   | $C_{w1}$ | $C_{w2}$    |
|---|----------|-------------|
| Das Sarma and Mason <sup>58</sup>         | $-\pi/2$ | $-0.062$    |
| Feynman's theory <sup>59</sup>            | $-\pi/2$ | $-0.04569$  |
| 4th, 6th order pert. theory <sup>59</sup> | $-\pi/2$ | $-0.06397$  |
| Hipolito <sup>60</sup>                    | $-\pi/2$ | $-0.0245$   |
| Present $E_0(\alpha)$                     | $-\pi/2$ | $-0.046626$ |
| Present $E_0(\alpha) + \Delta E_2$        | $-\pi/2$ | $-0.063974$ |

and

$$C_{w2} = -\frac{R_d^2 d}{36} \left( 1 - \frac{8}{3\pi} \right) - \frac{R_d^2 \Gamma(d/2) d^2}{9\pi^{3/2}} \sum_{n=2}^{\infty} \frac{(2n)! \Gamma(n+1/2)}{4^n (n!)^2 \Gamma(n+d/2)} B_n, \quad (83)$$

$$B_n = \int \int_1^{\infty} dx dy \frac{1}{(x+y)^2} \left[ \frac{1}{(x \cdot y)^{n+1/2}} + \frac{1}{(x+y-1)^{n+1/2}} \right].$$

For comparison, in Table I we give the known results for  $d=2$  as  $\alpha \rightarrow 0$ . One can see from Table I that our  $C_{w2}$  obtained only from  $E_0(\alpha)$  improves Feynman's estimate by about 2%. Addition of the next correction calculated from  $\Delta E_2$  results in  $C_{w2} = -0.063974$ , which is in good agreement with the exact value.<sup>54</sup> Note that  $\Delta E_2$  contributes about 40% to the total value of  $C_{w2}$ .

For three dimensions, the results are displayed in Table II together with the known results of the polaron GSE for the weak-coupling limit. Our leading term of the energy  $E_0(\alpha)$  improves the Feynman variational estimate of  $C_{w2}$  by 2%. The next correction results in  $C_{w2} = -0.015919$ , which is in good agreement with the exact value.<sup>54</sup> Note that for  $d=3$  our  $\Delta E_2$  contributes about 29% (smaller than for  $d=2$ ) to the total value of  $C_{w2}$ . Comparing the results for  $d=2$  and  $d=3$ , we conclude that the higher-order corrections (the second-order one in our case) coming from  $J_T(\alpha)$  are much more important for  $d=2$  than for  $d=3$ . In other words, the polaron effect is stronger in low space dimensions [see Eq. (80)]. This effect was noted earlier in Refs. 50 and 54.

TABLE II. Comparison of known weak-coupling results for the polaron ground-state energy  $E(\alpha) = \alpha \cdot C_{w1} + \alpha^2 \cdot C_{w2} + O(\alpha^3)$  in three dimensions.

| Authors                            | $C_{w1}$ | $C_{w2}$       |
|------------------------------------|----------|----------------|
| Das Sarma and Mason <sup>58</sup>  | $-1$     | $-0.016$       |
| Feynman's theory <sup>59</sup>     | $-1$     | $-0.012347$    |
| Röseler <sup>61</sup>              | $-1$     | $-0.0159196^*$ |
| Lee <i>et al.</i> <sup>52</sup>    | $-1$     | $-0.014$       |
| Larsen <sup>39</sup>               | $-1$     | $-0.016$       |
| Present $E_0(\alpha)$              | $-1$     | $-0.012598$    |
| Present $E_0(\alpha) + \Delta E_2$ | $-1$     | $-0.015919$    |

\* Exact value.

TABLE III. Comparison of estimates obtained for the coefficient  $C_s$  of the polaron ground-state energy  $E(\alpha) = \alpha^2 \cdot C_s + O(1)$  for  $d=2$  as  $\alpha \rightarrow \infty$ .

| Authors                               | $C_s$                  |
|---------------------------------------|------------------------|
| Das Sarma and Mason <sup>58</sup>     | -0.392699              |
| Feynman's theory <sup>59</sup>        | -0.392699 <sup>1</sup> |
| Xiaoguang <i>et al.</i> <sup>59</sup> | -0.4047 <sup>2</sup>   |
| Hipolito <sup>60</sup>                | -0.392699              |
| Present $E_0(\alpha)$                 | -0.392699              |
| Present $E_0(\alpha) + \Delta E_2$    | -0.400538              |

<sup>1</sup>Estimated in Ref. 59.

<sup>2</sup>Adiabatic approximation.

## B. Strong-coupling regime

The GSE of the polaron in the electron-phonon strong-coupling regime has been considered in Refs. 41 and 56–59.

It is well known that in this limit

$$E(\alpha) = \alpha^2 \cdot C_s + O(1). \quad (84)$$

For large  $\alpha$ , (75) becomes

$$E^{(2)}(\alpha) = -\alpha_d^2 \left\{ \frac{d}{9\pi} + \frac{2\Gamma(d/2)d^2}{9\pi^{3/2}} \times \sum_{n=2}^{\infty} \frac{(2n)!\Gamma(n+1/2)}{16^n(n!)^2 n\Gamma(n+d/2)} \right\} + O(1). \quad (85)$$

For comparison, in Table III we give our result together with the known results of the polaron GSE for  $d=2$  in the strong-coupling regime  $\alpha \rightarrow \infty$ .

For three dimensions the estimate of the next higher-order corrections for the coefficient  $C_s$  was obtained by the present authors earlier in Ref. 56:

$$C_s \leq -0.108431. \quad (86)$$

A comparison of the known results for the coefficient  $C_s$  for  $d=3$  is displayed in Table IV.

## C. Intermediate-coupling range

In the intermediate-coupling regime the main tool for obtaining polaron properties is the variational approach.<sup>35,52</sup> For  $d=3$ , the Feynman variational method based on a trial

TABLE IV. Comparison of estimates obtained for the coefficient  $C_s$  of the polaron ground-state energy  $E(\alpha) = \alpha^2 \cdot C_s + O(1)$  for  $d=3$  as  $\alpha \rightarrow \infty$ .

| Authors                               | $C_s$                  |
|---------------------------------------|------------------------|
| Feynman and Schultz <sup>65</sup>     | -0.1061                |
| Pekar (by Miyake) <sup>41</sup>       | -0.108504 <sup>1</sup> |
| Miyake <sup>41</sup>                  | -0.108513 <sup>2</sup> |
| Luttinger and Lu <sup>62</sup>        | -0.1066                |
| Marshall and Mills <sup>67</sup>      | -0.1078                |
| Sheng and Dow <sup>68</sup>           | -0.1065                |
| Adamowski <i>et al.</i> <sup>57</sup> | -0.1085128             |
| Feranchuk and Komarov <sup>69</sup>   | -0.1078                |
| Efimov and Ganbold <sup>56</sup>      | -0.10843               |

<sup>1</sup>Estimated in Ref. 41.

<sup>2</sup>Exact value.

oscillator-type action gives an upper bound on the polaron free energy, valid for arbitrary  $\alpha$ . Generalizations of the Feynman action for  $d=3$  to an arbitrary density function<sup>42</sup> and an arbitrary quadratic action<sup>43</sup> have improved this upper bound. In our opinion, the result<sup>43</sup> obtained for  $d=3$  is the best variational upper bound in the whole range of  $\alpha$ . But this variational method does not give the next corrections to this bound. Other numerical methods dealing with this problem<sup>62,63</sup> require specific complicated schemes of calculations which may introduce statistical errors. The estimates of both the upper and lower bounds for the polaron self-energy obtained in Refs. 39 and 64 should be improved.

Considering intermediate values of  $\alpha$ , we have derived Eqs. (63) and (64) numerically, by the following iteration scheme:

$$F_{n+1}(t) = \Phi_L[\tilde{\Sigma}_n], \quad (87)$$

$$\tilde{\Sigma}_n(k) = \Omega_k[F_n], \quad n \geq 0,$$

starting from reasonable assumed functions  $F_0(t)$  and  $\tilde{\Sigma}_0(k)$  [see (70)]. Both of the series  $F_n(t)$  and  $\tilde{\Sigma}_n(k)$  turn out to be rapidly convergent, and the value of the leading term  $E_0(\alpha)$  does not change after  $n \geq 6$ . The results for  $E_0(\alpha)$  and  $E^{(2)}(\alpha)$  in two dimensions are presented in Table V.

The values of  $E_0(\alpha)$  and  $E^{(2)}(\alpha)$  for  $d=3$  are given in Table VI, in comparison with the known data.<sup>39,43,64,65</sup> Our  $E_0(\alpha)$  for  $d=3$  coincides with the upper bound obtained in Ref. 43 and improves the variational results calculated in Ref. 71.

We have made preliminary estimates which indicate that the decreasing series in (73) is alternating. Then one can expect that the third-order correction  $\Delta E_3(\alpha)$  may slightly increase the value of  $E^{(2)}(\alpha)$ , and inclusion of higher-order corrections  $\Delta E_{n>2}(\alpha)$  might result in an insignificant oscillation of  $E^{(n>2)}(\alpha)$  between  $E_0(\alpha)$  and  $E^{(2)}(\alpha)$ . In other words, the value obtained for  $E^{(2)}(\alpha)$  may be accepted as a lower bound on the ground-state energy of the polaron. Note that the numerical results obtained in Ref. 66 at three points ( $\alpha=1,3,5$ ) by the method of “partial averaging” lie exactly between our curves for  $E_0(\alpha)$  and  $E^{(2)}(\alpha)$ . Recent exact Monte-Carlo calculations<sup>72</sup> are in good agreement with our results for  $d=3$ .

Our results obtained with the proposed method provide a reasonable description of both two- and three-dimensional polarons for an arbitrary coupling  $\alpha$ . Our considerations could be extended to computing the other characteristics of the polaron, the effective mass and the average number of phonons, as well as to estimating the energy of the polaron in the presence of a magnetic field, in view of the validity of the proposed method for the complex functionals.

## 4. CHARACTER OF PHASE TRANSITION IN THE TWO- AND THREE-DIMENSIONAL $\varphi^4$ THEORY

The phenomenon of spontaneous symmetry breaking, or, in other words, the vacuum-structure rearrangement, is an important part of many quantum field constructions. In this section, we will investigate this phenomenon within the GER method. The problem, of course, can also be studied within the canonical-quantization method. However, the functional



TABLE V. Estimates obtained for the polaron ground-state energy  $E_0(\alpha)$  and  $E^{(2)}(\alpha)$  for  $d=2$  in the intermediate range of  $\alpha$ , compared with known results obtained in Refs. 58, 60, and 70.

| $\alpha$ | Feynman* | Hipolito <sup>60</sup> | Huybrecht <sup>70</sup> | Das Sarma <sup>58</sup> | Present |             |
|----------|----------|------------------------|-------------------------|-------------------------|---------|-------------|
|          |          |                        |                         |                         | $E_0$   | $E_0 + E_2$ |
| 0.6364   | -1.0198  | -1.0266                | -1.0201                 | -1.0405                 | -1.020  | -1.028      |
| 1.909    | -3.2247  | -3.2263                | -3.2263                 | -3.5690                 | -3.231  | -3.250      |
| 3.183    | -5.9191  | -6.0902                | -5.9193                 | -6.9688                 | -5.928  | -6.039      |
| 4.450    | -9.6935  | -9.8723                | -9.7154                 | -11.388                 | -9.710  | -9.871      |

\*Our estimation by Feynman's variational method.

representation has the advantage of calculating the whole effective potential (EP) in this theory, which allows one to obtain more information about the phase structure and phase transitions in the system under consideration.

#### 4.1. Statement of the problem

The scalar  $\varphi^4$  theory in two and three dimensions has been intensively investigated<sup>73,74</sup> as a simple but nontrivial example for which the problem of spontaneous symmetry breaking or, in other words, the phase structure of quantum field models is studied. It has been found<sup>75</sup> that the highest-order quantum corrections can give rise to instability of the classical symmetric vacuum. There are two phases in this system, and PT phenomena take place at certain coupling strengths. The most difficult problem here is to determine the order of the PT.

The simplest example in which the vacuum exhibits a nontrivial structure is the  $\varphi_2^4$  theory. Many papers<sup>73-76</sup> are devoted to investigation of the nature of the PT in this model. We briefly treat some nonperturbative methods that seem to be basic among the investigations on this subject. An original approximation<sup>73</sup> using a Hartree-type renormalization exhibits a first-order PT in this theory. A similar result was obtained<sup>77</sup> within the Gaussian EP approach. The dimensionless critical coupling constant for which the first-order phase transition takes place is  $G=1.62$  in both papers. These con-

clusions disagree with mathematical theorems<sup>83,84</sup> proving that a second-order PT should occur in the  $\varphi_2^4$  model. There are papers<sup>76-85</sup> in which different variational methods have been used for solving this problem and a second-order PT has been observed in the region  $G \sim 1$ . In previous studies,<sup>88,89</sup> we have shown that the critical coupling constant leading to a second-order PT cannot exceed the value  $G_0=1.4392$  and may be found near  $G_{\text{crit}} \sim 0.53$ .

We study this problem by using the method of the EP. The absolute minimum of the EP  $V(\varphi_0)$  at the point  $\varphi_0=\varphi_c$  determines the true ground state (vacuum) of the theory. If a PT takes place at a certain coupling  $g=g_c$ , then for  $g < g_c$  the system is still in the original unbroken-symmetry phase with  $\varphi_c=0$ . On reaching  $g=g_c$  the origin  $\varphi_0=0$  is no longer the absolute minimum of  $V(\varphi_0)$ , and the system goes to a new state with  $\varphi_c \neq 0$  corresponding to lower energy. The first-order PT means that the point  $\varphi=0$  remains local, but is not the absolute minimum of  $V(\varphi_0)$ . In other words, the first derivative of  $V(\varphi_0)$  is zero, and the second one is positive at the origin  $\varphi_0=0$ . In the case of the second-order transition, the point  $\varphi_0=0$  is a local maximum of the EP at  $g > g_c$ . The second derivative of  $V(\varphi_0)$  at  $\varphi_0=0$  becomes negative. Thus, the coefficient  $\alpha(g)$  in the representation of  $V(\varphi_0)$  for small  $\varphi_0$ ,

$$V(\varphi_0) = E(g) + \alpha(g) \cdot \varphi_0^2 + O(\varphi_0^4), \quad (88)$$

TABLE VI. Estimates obtained for the polaron ground-state energy  $E_0(\alpha)$  and  $E^{(2)}(\alpha)$  for  $d=3$  in the intermediate range of  $\alpha$ , compared with known results obtained in Refs. 39, 57, 64, and 65.

| $\alpha$ | Osc. <sup>57</sup> | Feynman <sup>65</sup> | Smondyrev <sup>64</sup> |         | Larsen <sup>39</sup> |         | Present |             |
|----------|--------------------|-----------------------|-------------------------|---------|----------------------|---------|---------|-------------|
|          | upper              | upper                 | upper                   | lower   | upper                | lower   | $E_0$   | $E_0 + E_2$ |
| 0.5      | -0.5               | -0.5032               | -0.5041                 | -0.5041 | -0.5040              | -0.5052 | -0.504  | -0.5041     |
| 1.0      | -1.0               | -1.0130               | -1.0167                 | -1.0175 | -1.0160              | -1.0270 | -1.014  | -1.017      |
| 1.5      | -1.5               | -1.5302               | -                       | -       | -1.5361              | -1.576  | -1.532  | -1.539      |
| 2.0      | -2.0               | -2.0554               | -                       | -       | -2.0640              | -2.172  | -2.058  | -2.071      |
| 2.5      | -2.5               | -2.5894               | -                       | -       | -2.5995              | -2.872  | -2.593  | -2.614      |
| 3.0      | -3.0               | -3.1333               | -3.1645                 | -3.2122 | -3.1421              | -       | -3.138  | -3.167      |
| 4.0      | -4.0               | -4.2565               | -                       | -       | -4.2771              | -       | -4.265  | -4.305      |
| 5.0      | -5.0               | -5.4401               | -5.4945                 | -5.7767 | -                    | -       | -5.452  | -5.528      |
| 7.0      | -7.356             | -8.1127               | -8.0406                 | -8.8832 | -                    | -       | -8.137  | -8.255      |
| 9.0      | -10.72             | -11.486               | -10.834                 | -12.654 | -                    | -       | -11.54  | -11.69      |
| 11.0     | -14.94             | -15.710               | -13.905                 | -17.165 | -                    | -       | -15.83  | -16.04      |
| 20.0     | -44.53             | -45.283               | -                       | -       | -                    | -       | -45.33  | -45.99      |
| 30.0     | -97.58             | -98.328               | -                       | -       | -                    | -       | -98.52  | -99.86      |
| 40.0     | -171.9             | -172.60               | -                       | -       | -                    | -       | -173.4  | -175.1      |

plays an important role in the determination of the character of the phase transition. If  $\alpha(g)$  is zero at a certain  $g=g_c$  and negative for  $g>g_c$  up to  $g\rightarrow\infty$ , then one can say that a second-order PT appears here. On the contrary, positiveness of  $\alpha(g)$  for any  $g$  excludes a second-order transition. Rigorous calculation of  $\alpha(g)$  for an arbitrary coupling constant is a complicated problem. However, we know that at large  $g$  the coefficient  $\alpha(g)$  remains negative in the case of a second-order PT and is positive if the transition is of first order.

We study this problem qualitatively by using the GER method described in Sec. 2.1. We will show the possibility of a second-order PT in the  $g\varphi_2^4$  theory and give an estimate for the corresponding critical coupling constant  $g_c$ . For the  $g\varphi_3^4$  model our result excludes the occurrence of a second-order phase transition.

## 4.2. Renormalized Lagrangian of the $\varphi_{2,3}^4$ model

We consider the  $g\varphi^4$  scalar-field model in two and three dimensions. We will use throughout this section the Euclidean form of the model.<sup>1)</sup> This theory contains ultraviolet divergences, but it is super-renormalizable, i.e., it has only a finite number of divergent Feynman diagrams. In order to remove these divergences, we must introduce appropriate counterterms in the Lagrangian. In this section we consider the super-renormalized scalar field theory with the Lagrangian

$$L = \frac{1}{2} \varphi(x) [\partial^2 - m^2] \varphi(x) - \frac{g}{4} N_m \{ \varphi^4(x) \} - R_m, \quad (89)$$

where we have introduced a "normal-ordered" form of interaction as follows:

$$N_m \{ \varphi^4(x) \} = \varphi^4(x) - 6\varphi^2(x)D_m(0) + 3D_m^2(0),$$

$$D_m(x) = \int \frac{d^d k}{(2\pi)^d} \frac{\exp\{ikx\}}{m^2 + k^2}. \quad (90)$$

Here  $x \in \Omega$ , where  $\Omega$  is a large but finite volume in  $R^d$  ( $d=2,3$ ), and  $m$  and  $g$  are the mass and the self-coupling constants, respectively. In two dimensions ( $d=2$ ) all the divergences are only of the "tadpole" type and are readily removed by introducing the normal product  $N_m$  of the fields  $\varphi(x)$  in (89). In this case  $R_m=0$ . In the three-dimensional theory there are additional divergences, which are canceled by counterterms

$$R_m = \frac{1}{2} A_m N_m \{ \varphi^2(x) \} + \delta E_m, \quad (91)$$

where

$$\begin{aligned} A_m &= 6g^2 \int d^3x D_m^3(x), \\ \delta E_m &= \frac{3}{4} g^2 \int d^3x D_m^4(x) \\ &\quad - \frac{3}{2} g^3 \int \frac{d^3k}{(2\pi)^3} \left\{ \int d^3x e^{ikx} D_m^2(x) \right\}^3. \end{aligned} \quad (92)$$

At small  $g$  the Lagrangian (89) describes a system that is invariant with respect to the transformation  $\varphi \leftrightarrow -\varphi$ . The question is whether this symmetry remains for increasing  $g$ .

## 4.3. Effective potential in the $\varphi_{2,3}^4$ theory

The EP is defined as

$$V(\varphi_0) = - \lim_{\Omega \rightarrow \infty} \frac{1}{\Omega} \ln I_\Omega(\varphi_0),$$

$$I_\Omega(\varphi) = C_m \int \delta\varphi \delta \left\{ \varphi - \frac{1}{\Omega} \int d^d x \varphi(x) \right\} \exp \int_\Omega d^d x L[\varphi(x)],$$

$$C_m = \sqrt{\det\{-\partial^2 + m^2\}}. \quad (93)$$

All the integrations are performed in the Euclidean metric.

According to the GER method, we transform the field variable as

$$\varphi(x) = \phi_0 + b(x) + \phi(x), \quad (94)$$

where the new field variable  $\phi(x)$  corresponding to the new mass  $\mu$  and the function  $b(x)$  satisfy the conditions

$$\int_\Omega d^d x \phi(x) = 0, \quad \int_\Omega d^d x b(x) = 0, \quad b^2(x) = b^2 = \text{const}. \quad (95)$$

Let us go over to the normal ordering in the new fields  $\phi(x)$ , using the well-known formula<sup>75</sup>

$$N_m \{ \exp\{\beta\varphi(x)\} \} = N_\mu \left\{ \exp \left\{ \beta(\phi_0 + b(x) + \phi(x)) + \frac{\beta^2}{2} \Delta(m, \mu) \right\} \right\},$$

$$\Delta = \Delta(m, \mu) = D_m(0) - D_\mu(0),$$

$$D_\mu(x) = \int \frac{d^d k}{(2\pi)^d} \frac{\exp\{ikx\}}{\mu^2 + k^2} - \frac{1}{\mu^2 \Omega}. \quad (96)$$

First we substitute (94) and (96) into (93) and perform the integration over  $d\phi_0$ . Then, following the key steps of the GER method, we obtain

$$\begin{aligned} I_\Omega(\varphi_0) &= e^{-\Omega V_0(\varphi_0)} \int d\sigma_\mu \exp \left\{ \int_\Omega d^d x N_\mu \left[ \frac{g}{4} [\phi^4(x) + 4\phi^3(x)(\phi_0 + b(x)) + 12\phi_0 b(x)\phi^2(x)] \right. \right. \\ &\quad \left. \left. - \left[ \frac{1}{2} A_\mu \phi^2(x) + A_\mu b(x)\phi(x) + \delta E_\mu + \frac{1}{2} (b^2 + \varphi_0^2) A_\mu \right] \right] \right\}, \\ \int d\sigma_\mu \cdot 1 &= C_\mu \int \delta\phi \exp \left\{ -\frac{1}{2} \int_\Omega d^d x \phi(x) \times (-\partial^2 + \mu^2) \phi(x) \right\} = 1, \end{aligned} \quad (97)$$

where the new counterterms concentrated in the second square brackets in (97) coincide with (92) if we substitute  $m \rightarrow \mu$ . The leading-order term of the EP is obtained as the “cactus”-type part  $V_0(\varphi_0)$  of the EP as follows:

$$V_0(\varphi_0) = -\frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \left[ \ln \left( 1 + \frac{m^2 - \mu^2}{\mu^2 + k^2} \right) - \frac{m^2 - \mu^2}{\mu^2 + k^2} \right] + \frac{m^2}{2} (\varphi_0^2 + b^2) + \frac{g}{4} (\varphi_0^4 + 6\varphi_0^2 b^2 + b^4) - 6\Delta(\varphi_0^2 + b^2) + 3\Delta^2 + \frac{\varphi_0^2 + b^2}{2} (A_m - A_\mu) + \left( \delta E_m - \delta E_\mu - \frac{1}{2} A_m \Delta \right). \quad (98)$$

The requirement that the linear term  $N_\mu\{\phi\}$  must not arise in the interaction and that the quadratic field configurations be concentrated in the Gaussian measure  $d\sigma_\mu$  leads to the following constraint equations for the parameters  $b(x)$  and  $\mu$ :

$$b(x)[-m^2 + 3g(\Delta - \varphi_0^2) - gb^2 - A_m + A_\mu] = 0, \quad \mu^2 - m^2 + 3g(\Delta - \varphi_0^2 - b^2) - A_m + A_\mu = 0. \quad (99)$$

Thus, we finally obtain the formula for the effective potential:

$$V(\varphi_0) = V_0(\varphi_0) + V_{sc}(\varphi_0), \quad V_{sc}(\varphi_0) = -\lim_{\Omega \rightarrow \infty} \frac{1}{\Omega} \ln J_\Omega(\varphi_0), \quad (100)$$

where a new path integral is introduced in the form

$$J_\Omega(\varphi_0) = e^{-\Omega V_{sc}(\varphi_0)} = \int d\sigma_\mu \exp \left\{ \int_\Omega d^d x \times N_\mu \times \left[ -\frac{g}{4} [\phi^4(x) + 4\phi^3(x)(\varphi_0 + b(x)) + 12\varphi_0 b(x)\phi^2(x)] - \left[ \frac{1}{2} A_\mu \phi^2(x) + A_\mu b(x)\phi(x) + \delta E_\mu + \frac{1}{2} (b^2 + \varphi_0^2) A_\mu \right] \right] \right\}. \quad (101)$$

Equations (98) and (99)–(101) define completely the EP for an arbitrary coupling  $g$ . Below, we will investigate the EP in (100), whose parameters  $b(x)$  and  $\mu$  are restricted by the constraints (96).

For further consideration, it will be convenient to work in units of  $m$  when dealing with numerical results. We define

$$\xi = (\mu/m)^{4-d}, \quad \Phi_0^2 = 4\pi m^{2-d} \varphi_0^2, \quad \text{and} \quad B^2 = 4\pi m^{2-d} b^2. \quad (102)$$

#### 4.4. The “cactus”-type potential as the leading-order term of the effective potential

In two dimensions, the “cactus-type” part of the EP becomes

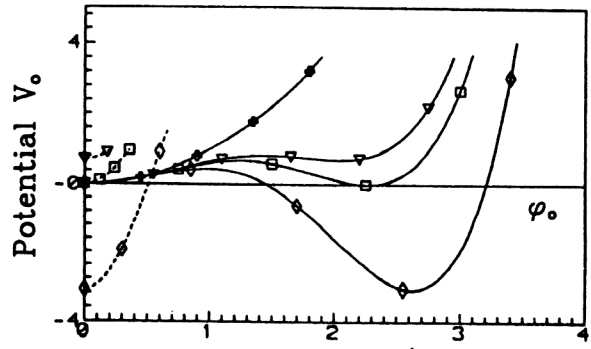


FIG. 3. The Gaussian part  $V_0(\Phi_0)$  (in units of  $m^2/8\pi$ ) of the effective potential as a function of  $\Phi_0$  for different values of the coupling constant: crosses,  $G=0.5$ ; triangles,  $G=1.5$ ; squares,  $G=1.6251$ ; diamonds,  $G=2.0$ . The dashed lines represent the “nontrivial” branches. The “trivial” branches are denoted by the solid lines.

$$V_0(\Phi_0) = \frac{m^2}{8\pi} \left\{ \xi - 1 - \ln \xi + \Phi_0^2 + B^2 + \frac{G}{4} [\Phi_0^4 + B^4 + 3 \ln^2 \xi + 6(B^2 \Phi_0^2 - B^2 \ln \xi - \Phi_0^2 \ln \xi)] \right\}. \quad (103)$$

We note that the potential (103) is invariant for  $\Phi_0 \leftrightarrow B$ .

The parameters  $\xi$  and  $B$  in (103) are restricted by the following equations:

$$\begin{cases} B^2(\xi - GB^2) = 0, \\ 2\xi - 2 + 3G(\ln \xi - \Phi_0^2 - B^2) = 0. \end{cases} \quad (104)$$

Let us consider the constraint (104). A pair of “trivial” solutions

$$B=0 \quad \text{and} \quad \xi = 1 - \frac{3G}{2} (\ln \xi - \Phi_0^2) \quad (105)$$

can be found for an arbitrary coupling constant  $G$ . Since  $G > G_0 = 1.4392$ , an additional pair of “nontrivial” solutions

$$B = \frac{\xi}{G} \quad \text{and} \quad \xi = -2 + \frac{3G}{2} (\ln \xi - \Phi_0^2) \quad (106)$$

also appears here. Thus, for  $G < G_0$  the only solution to be substituted into (103) is the “trivial” one, but since  $G > G_0$ , there is an alternative: one can choose either (105) or (106). We choose the pair with the lowest value of  $V_c(\Phi_0)$  for some fixed  $\Phi_0$ .

All the necessary calculations can be performed numerically. The resulting potential  $V_c(\Phi_0)$  is plotted in Fig. 3. Near the origin  $\Phi_0=0$  the potential  $V_c(\Phi_0)$  is represented by the “nontrivial” branch (if  $G > G_0$ )  $B \neq 0$ , as it is situated below the “trivial” one. But for larger values of  $\Phi_0$  the “trivial” solution  $B=0$  provides the lowest value of the potential. This picture leads to an interesting result. Let us consider the local minima of both branches. For  $B=0$  the minimum point  $\Phi_0=A$  in Fig. 3 is given by the equations

$$\begin{cases} B=0, \\ 2 - 3G \ln \xi + G\Phi_0^2 = 0. \end{cases} \quad (107)$$

On the other hand, the minimum of the “nontrivial” branch  $B \neq 0$  is fixed at the origin  $\Phi_0 = 0$  for any  $G > G_0$ , and (104) becomes

$$\begin{cases} \Phi_0 = 0, \\ 2 - 3G \ln \xi + GB^2 = 0. \end{cases} \quad (108)$$

Owing to the invariance of the potential  $V_c(\Phi_0, B)$  in (103) for  $\Phi_0 \leftrightarrow B$ , our expressions (107) and (108) are identical. In other words, the minima of the potential (103) corresponding to different solutions of (104) are equal. The vacuum with  $\langle \Phi(x) \rangle = \Phi_0 \neq 0$  is not lower than the initial one located at the point  $\langle \Phi(x) \rangle = \Phi_0 = 0$ . There is no reason for the occurrence of a first-order phase transition.

#### 4.5. Non-Gaussian correction in the $\varphi_2^4$ model

In the previous section, we derived an expression for the EP consisting of two parts. Considering only the “leading” term  $V_0(\varphi_0)$ , one can say nothing about the nature of the PT in the theory. To answer this question one must also consider the remaining part  $V_{sc}(\varphi_0)$  of the effective potential, defined in (100). In the weak-coupling limit one can estimate it by expanding the exponential in (97) in a perturbative series. But explicit calculation of the non-Gaussian functional integral  $J_\Omega(\varphi_0)$  in (97) for arbitrary values of the coupling constant  $g$  and  $\varphi_0$  is a complicated problem. However, we are able to estimate it for infinitesimal values of  $\varphi_0$  for arbitrary  $g$ .

We rewrite (97) in a form that is correct for infinitesimal  $\varphi_0$ :

$$\begin{aligned} J_\Omega(\varphi_0) = \int d\sigma_\mu \exp \left\{ -\frac{g}{4} \int_\Omega d^d x N_\mu [\phi^4(x) \right. \\ \left. + 4b(x)\phi^3(x)] + \frac{g^2 \varphi_0^2}{2} \left[ \int_\Omega d^d x N_\mu (\phi^3(x) \right. \right. \\ \left. \left. + 3b(x)\phi^2(x)) \right]^2 \right\}. \end{aligned} \quad (109)$$

This representation can easily be obtained, in view of the validity of the following transformation in the integrand of (97):

$$\exp(-\varphi_0 W) = \cosh(\varphi_0 W) = \exp \left\{ \frac{1}{2} \varphi_0^2 W^2 + O(\varphi_0^4) \right\}$$

for infinitesimal  $\varphi_0$  and a finite functional  $W$ .

Applying to (109) Jensen's inequality, we get an upper bound

$$\begin{aligned} V_{sc}(\varphi_0) \leq V_{sc}^+(\varphi_0) = \\ -\frac{g^2 \varphi_0^2}{2\Omega} \int_\Omega d^d x \int_\Omega d^d y \int d\sigma_\mu \{ N_\mu \phi^3(x) N_\mu \phi^3(y) \\ + 9b(x)b(y) N_\mu \phi^2(x) N_\mu \phi^2(y) \}. \end{aligned} \quad (110)$$

It is easy to show that

$$\begin{aligned} \int d\sigma_\mu N_\mu \phi^3(x) N_\mu \phi^3(y) &= 6D_\mu^3(x-y), \\ \int d\sigma_\mu N_\mu \phi^2(x) N_\mu \phi^2(y) &= 2D_\mu^2(x-y). \end{aligned} \quad (111)$$

Then we rewrite (110) in the form

$$\begin{aligned} V_{sc}^+(\Phi_0) &= -\frac{m^2}{8\pi} \frac{3G^2 \Phi_0^2}{2\xi} (Q + 3B^2), \\ Q &= \frac{4\pi \ln 2}{3\sqrt{3}} - 4 \int_0^1 \frac{du}{u^2 + 3} \ln(1 - u^2) = 2.3439 \dots \end{aligned} \quad (112)$$

Substituting the parameters  $\xi$  and  $B$  in either (105) or (106) into (112), we find the behavior of  $V_{sc}^+(\Phi_0)$  for small values  $\Phi_0 \sim 0$ . Omitting the details of the calculations, we write the results:

$$V_{sc}^+(\Phi_0) = -\frac{m^2}{8\pi} \left\{ -\frac{3Q}{2} G^2 \Phi_0^2 + O(\Phi_0^4) \right\} \quad \text{for } G < G_* \quad (113)$$

and

$$\begin{aligned} V_{sc}^+(\Phi_0) &= -\frac{m^2}{8\pi} \left\{ -\left[ \frac{3QG^2}{2\xi} + \frac{9G}{2} \right] \Phi_0^2 \right. \\ &\quad \left. + O(\Phi_0^4) \right\} \quad \text{for } G > G_*, \\ 3G \ln \xi - \xi - 2 &= 0. \end{aligned} \quad (114)$$

From (103) we get the following asymptotic behavior:

$$V_0(\Phi_0) = \frac{m^2}{8\pi} \{ \Phi_0^2 + O(\Phi_0^4) \} \quad (115)$$

as  $\Phi_0 \rightarrow 0$  for any  $G$ .

Finally, taking into account (100), we obtain the following behavior of the upper bound for the EP in the region of small  $\Phi_0 \sim 0$ :

$$\begin{aligned} V^+[\Phi_0] &= V_0[\Phi_0] + V_{sc}^+[\Phi_0] \\ &= \frac{m^2}{8\pi} [\alpha(G) \Phi_0^2 + O(\Phi_0^4)], \end{aligned} \quad (116)$$

where

$$\begin{aligned} \alpha(G) &= \begin{cases} \alpha_1(G) = 1 - 3QG^2/2, & G \leq 1.6251, \\ \alpha_2(G) = 1 - 3QG^2/(2\xi) - 9G/2, & G > 1.6251, \end{cases} \\ 3G \ln \xi - \xi - 2 &= 0. \end{aligned} \quad (117)$$

One can easily check that the coefficient  $\alpha_1(G)$  in (117) becomes negative for  $G > G_{\text{crit}} = 0.5333$  and remains negative for increasing  $G$ . But  $\alpha_2(G)$  is negative at arbitrary  $G > 1.4392$ . In our opinion, this indicates the occurrence of a second-order PT in the model under consideration.

#### 4.6. Strong-coupling regime in the $\varphi_3^4$ model

In the three-dimensional case the counterterms defined by (92) play an important role in the behavior of the EP in the strong-coupling regime. We have

$$D_m(x) = \frac{\exp\{-\mu|x|\}}{4\pi|x|}, \quad \Delta = \frac{m}{4\pi} (\xi - 1). \quad (118)$$

Substituting (118) into (99), we get

$$B(x)[2 + 3G(\Phi_0^2 - \xi + 1) + GB^2 + 3G^2 \ln \xi] = 0, \\ -2\xi^2 + 2 + 3G(\Phi_0^2 - \xi + 1) + 3GB^2 + 3G^2 \ln \xi = 0. \quad (119)$$

A nontrivial solution  $B \neq 0$  exists only for  $0 < \xi < 1$ . Let us consider the solution  $B = 0$ . In the strong-coupling regime we obtain

$$\xi = G \sqrt{\frac{3}{G} \ln G + O(G \sqrt{\ln \ln G})}. \quad (120)$$

In other words, the effective coupling constant

$$G_{\text{eff}} = \frac{g}{2\pi\mu} = \frac{G}{\xi} = \sqrt{\frac{2}{3 \ln G}} \left\{ 1 + O\left(\frac{\ln \ln G}{\ln G}\right) \right\} \quad (121)$$

is small for  $G \rightarrow \infty$ , and we are actually dealing with the weak-coupling regime. This means that the effective coupling constant

$$G_{\text{eff}} = \frac{g}{2\pi\mu^2} = \frac{G}{\xi} = \frac{1}{3 \ln G} \left\{ 1 + O\left(\frac{\ln \ln G}{\ln G}\right) \right\} \quad (122)$$

becomes small for  $G \rightarrow \infty$ , and one can successfully develop a perturbation expansion in  $G_{\text{eff}}$  for the functional integral (101):

$$V_{\text{sc}}(\varphi_0) = \sum_{n=1}^{\infty} G_{\text{eff}}^n V_{\text{sc}}^{(n)}(\varphi_0). \quad (123)$$

Here  $V_{\text{sc}}^{(1)} = 0$ , owing to the normal ordering in the exponent in (101). After some calculations we obtain

$$V_{\text{sc}}^{(1)}(\varphi_0) = V_{\text{sc}}^{(2)}(\varphi_0) = 0, \\ V_{\text{sc}}^{(3)}(\varphi_0) = \frac{m^3}{8\pi} \frac{18C_1}{\xi} G^3 \Phi_0^2, \quad (124)$$

where the constant is

$$C_1 = \frac{1}{2\pi^6} \int \int \int \frac{d^3k d^3p d^3q}{(1+k^2)(1+p^2)(1+q^2)(1+(k+p)^2)(1+(k+q)^2)} \\ \times \frac{16}{\pi} \int_0^\infty \frac{du}{1+4u^2} (\arctan u)^2 = 1.7593 \dots$$

Taking into account the ‘‘cactus’’-type potential

$$V_0(\Phi_0) = \frac{m^3}{8\pi} \left\{ E_0(G) + \frac{3G}{2} (G \ln \xi - \xi) \Phi_0^2 + O(\Phi_0^4) \right\}, \quad (125)$$

we finally obtain the effective potential

$$V(\Phi_0) = V_0(\Phi_0) + V_{\text{sc}}(\Phi_0) \\ = \frac{m^3}{8\pi} \{E(G) + \alpha \Phi_0^2 + O(\Phi_0^4)\}, \quad (126)$$

where the desired coefficient

$$\alpha(G) = \frac{3G^2}{2} \ln G \left\{ 1 + \frac{\sqrt{96}C_1}{(\ln G)^{3/2}} + O\left(\frac{1}{(\ln G)^{5/2}}\right) \right\} \quad (127)$$

is positive. This result excludes second-order phase transitions in the  $\varphi_3^4$  model. This can be accepted as an argument in favor of either the existence of only a first-order transition or the absence of any PT in the three-dimensional case.

Comparing the results (117) and (127) for  $d=2$  and  $d=3$ , we find that the effective mass renormalization is crucial for this problem. In two dimensions the mass renormalization includes ‘‘tadpole’’ divergences only, and the behavior of  $\alpha(G)$  in (117) favors a second-order PT in  $\varphi_2^4$ . For  $d=3$  the mass renormalization contains an additional term of the second perturbative order which has the opposite sign from a ‘‘tadpole’’ contribution. As a result, the function  $\alpha(G)$  in (127) remains positive for all  $G > 0$ .

#### 5. WAVE PROPAGATION IN RANDOMLY DISTRIBUTED MEDIA

The theoretical investigation of the propagation properties of waves in a randomly distributed environment reflects certain interest due to its many practical applications, including calculations of electronic conductance in crystals,<sup>90</sup> wave localization,<sup>91</sup> and dumping of signals in the atmosphere or in water.<sup>92</sup> A series of different methods has been applied to this problem, among which path-integral techniques<sup>93–95</sup> are of considerable interest.

In this section we investigate wave transmission in randomly distributed media, using the GER method.

##### 5.1. The Green function of the wave equation

The propagation of a wave  $u(\mathbf{x})$  (e.g., electromagnetic) in a time-independent environment can be described by the wave equation given in real 3-dimensional space  $\mathbf{x} \in R^3$ :

$$[\Delta + \omega^2(1 + \varepsilon(\mathbf{x}))]u(\mathbf{x}) = J(\mathbf{x}), \\ \omega \neq 0. \quad (128)$$

The notation is as follows. The constant  $\omega$  is the ‘‘dielectric constant’’ and defines the frequency of unperturbed waves;  $J(\mathbf{x})$  is the source function.

The random noise is described by a random stationary field  $\varepsilon(\mathbf{x})$  which is assumed to vary stochastically with a certain correlation function  $\langle \varepsilon(\mathbf{x})\varepsilon(\mathbf{y}) \rangle$ . For simplicity we shall consider the Gaussian noise

$$\langle \varepsilon(\mathbf{x})\varepsilon(\mathbf{y}) \rangle_\varepsilon = \lambda P(\mathbf{x} - \mathbf{y}) = \lambda \exp\left(-\frac{(\mathbf{x} - \mathbf{y})^2}{4l^2}\right) \\ = \lambda \int \frac{d\mathbf{k}}{\pi^{3/2}} \cdot \exp\left\{-\mathbf{k}^2 + i\mathbf{k} \frac{\mathbf{x} - \mathbf{y}}{l}\right\}, \quad (129)$$



where the interaction coefficient  $\lambda$  describes the intensity of the noise given by the distribution function  $P(\mathbf{x}-\mathbf{y})$  with a correlation length  $l$ . These two constants define the influence of the Gaussian noise on the propagation of waves in media.

The solution of (128) can be represented in the form

$$u(\mathbf{x}|\varepsilon) = \int d\mathbf{y} G(\mathbf{x}, \mathbf{y}|\varepsilon) J(\mathbf{y}), \quad (130)$$

where  $G(\mathbf{x}, \mathbf{y}|\varepsilon)$  is the Green function of the wave equation (128):

$$[\Delta + \omega^2(1 + \varepsilon(\mathbf{x}))]G(\mathbf{x}, \mathbf{y}|\varepsilon) = \delta(\mathbf{x} - \mathbf{y}). \quad (131)$$

The problem is to find the solution of (128) and then average it over the random fields  $\varepsilon(\mathbf{x})$  to find the wave amplitude:

$$u(\mathbf{x}) = \langle u(\mathbf{x}|\varepsilon) \rangle_\varepsilon. \quad (132)$$

For this the Green function must be averaged over the random fields  $\varepsilon(\mathbf{x})$ :

$$G(\mathbf{x} - \mathbf{y}) = \langle G(\mathbf{x}, \mathbf{y}|\varepsilon) \rangle_\varepsilon. \quad (133)$$

Thus, we consider this problem solved if the averaged Green function  $G(\mathbf{x})$  is found and its asymptotic behavior for large distance  $|\mathbf{x}| \rightarrow \infty$  can be calculated.

Let us proceed to solve Eq. (131) for the Green function. It is essential that the operator

$$K = \Delta + \omega^2(1 + \varepsilon(\mathbf{x})) \quad (134)$$

is not positive definite. We shall consider the solution

$$G(\mathbf{x}, \mathbf{y}|\varepsilon) = \frac{1}{K + i0} \delta(\mathbf{x} - \mathbf{y}), \quad (135)$$

corresponding to the so-called causal Green function. This solution can be written in the integral representation

$$\begin{aligned} G(\mathbf{x}, \mathbf{y}|\varepsilon) &= -\frac{i}{2} \int_0^\infty du e^{i/2(K+i0)u} \cdot \delta(\mathbf{x} - \mathbf{y}) \\ &= -\frac{i}{2} \int_0^\infty du T_\tau \exp \left\{ \frac{i}{2} \int_0^u d\tau \left[ \left( \frac{\partial}{\partial \mathbf{x}_\tau} \right)^2 \right. \right. \\ &\quad \left. \left. + \omega^2(1 + \varepsilon(\mathbf{x}_\tau)) \right] \right\} \delta(\mathbf{x} - \mathbf{y}), \end{aligned} \quad (136)$$

where we have used the "time-ordering" operator  $T_\tau$ . Repeating all the calculations of Sec. 2.8, which will be omitted here, we obtain

$$\begin{aligned} G(\mathbf{x}, \mathbf{y}|\varepsilon) &= -\frac{1}{2} \int_0^\infty \frac{du}{(2\pi i u)^{3/2}} \exp \left[ -\frac{i}{2} \left( \omega^2 u \right. \right. \\ &\quad \left. \left. + \frac{(\mathbf{x} - \mathbf{y})^2}{u} \right) \right] \cdot I_u(\mathbf{x}, \mathbf{y}|\varepsilon), \end{aligned} \quad (137)$$

where a FI is introduced:

$$\begin{aligned} I_u(\mathbf{x}, \mathbf{y}|\varepsilon) &= \int d\sigma_0 \exp \left\{ \frac{i}{2} \omega^2 \int_0^u d\tau \varepsilon \left( \mathbf{x} \frac{\tau}{u} + \mathbf{y} \left( 1 - \frac{\tau}{u} \right) \right. \right. \\ &\quad \left. \left. + \nu(\tau) \right) \right\}, \end{aligned} \quad (138)$$

with the measure defined as

$$d\sigma_0 = C_0 \delta\nu \exp \left\{ \frac{i}{2} \int_0^u d\tau \dot{\nu}^2(\tau) \right\}. \quad (139)$$

The integration in (138) is taken over "paths"  $\nu$  obeying the condition

$$\nu(0) = \nu(u) = 0.$$

Here the normalization is chosen so that the following condition is satisfied:

$$\int d\sigma_0 \cdot 1 = 1 \quad \text{or} \quad I_u(\mathbf{x}, \mathbf{y}|\varepsilon)|_{\varepsilon=0} = 1. \quad (140)$$

Now we can average the functional  $I_u(\mathbf{x}, \mathbf{y}|\varepsilon)$  over the random fields  $\varepsilon(\mathbf{x})$ :

$$\begin{aligned} I_u(\mathbf{x} - \mathbf{y}) &= \langle I_u(\mathbf{x}, \mathbf{y}|\varepsilon) \rangle_\varepsilon = \int d\sigma_0 \\ &\times \exp \left\{ -\lambda \frac{\omega^4}{8} \int_0^u \int_0^u d\tau d\tau' P \left( \nu(\tau) - \nu(\tau') \right. \right. \\ &\quad \left. \left. + (\mathbf{x} - \mathbf{y}) \frac{\tau - \tau'}{u} \right) \right\}. \end{aligned} \quad (141)$$

The averaged Green function is

$$G(\mathbf{x}) = -\frac{1}{2} \int_0^\infty \frac{du}{(2\pi i u)^{3/2}} \exp \left[ \frac{i}{2} \left( \omega^2 u + \frac{\mathbf{x}^2}{u} \right) \right] \cdot I_u(\mathbf{x}), \quad (142)$$

where

$$\begin{aligned} I_u(\mathbf{x}) &= C_0 \int_{\nu(0)=\nu(u)=0} \delta\nu \exp \left\{ \frac{i}{2} \int_0^u d\tau \dot{\nu}^2(\tau) \right. \\ &\quad \left. - \lambda \frac{\omega^4}{8} \int_0^u \int_0^u d\tau d\tau' P \left( \nu(\tau) - \nu(\tau') \right. \right. \\ &\quad \left. \left. + \mathbf{x} \frac{\tau - \tau'}{u} \right) \right\}. \end{aligned} \quad (143)$$

For further convenience we introduce the notation

$$\begin{aligned} r &= |\mathbf{x}|, \quad u = \frac{r}{\omega} z, \quad \beta = r\omega, \quad \tau = \frac{z}{\omega^2} t, \\ \tau' &= \frac{z}{\omega^2} s, \quad g = \frac{\lambda z^2}{4} \end{aligned} \quad (144)$$

and change the variable of the FI:

$$\nu(\tau) = \frac{\sqrt{z}}{\omega} \rho(t). \quad (145)$$

Then we have

$$\begin{aligned} G(\beta) &= -\frac{\omega}{2\sqrt{\beta}} \int_0^\infty \frac{dz}{(2\pi i z)^{3/2}} \\ &\times \exp \left[ i \frac{\beta}{2} \left( z + \frac{1}{z} \right) \right] \cdot I(\beta, z), \end{aligned} \quad (146)$$

where

$$I(\beta, z) = C_0 \int_{\rho(0)=\rho(\beta)} \delta\rho \exp \left\{ \frac{i}{2} \int_0^\beta dt \dot{\rho}^2(t) - \frac{g}{2} \int_0^\beta \int_0^\beta dt ds P \left( \frac{\sqrt{z}}{\omega} (\rho(t) - \rho(s)) + \mathbf{n} \frac{t-s}{\omega} \right) \right\}, \quad (147)$$

with

$$\mathbf{n} = \frac{\mathbf{x}}{|\mathbf{x}|}, \quad (\mathbf{n}\mathbf{n}) = 1.$$

## 5.2. The Green function at large distances

We now consider wave propagation for large distances  $\beta \rightarrow \infty$ . Then by analogy with the polaron problem, where similar asymptotics have been studied, we can expect the following behavior of the FI:

$$I(\beta, z) \sim \frac{1}{\beta^{O(1)}} \exp\{-\beta E(z; \lambda, \omega)\}. \quad (148)$$

Consequently,

$$G(\beta) \sim \frac{1}{\beta^{O(1)}} \int_0^\infty \frac{dz}{z^{3/2}} \exp \left\{ \beta \left[ \frac{i}{2} \left( z + \frac{1}{z} \right) - E(z; \lambda, \omega) \right] \right\} \sim \frac{1}{\beta^{O(1)}} \int_0^\infty \frac{dz}{z^{3/2}} \exp\{\beta S(z)\}, \quad (149)$$

where

$$S(z) = \frac{i}{2} \left( z + \frac{1}{z} \right) - E(z; \lambda, \omega).$$

The main contribution to the FI in (149) for large  $\beta$  can be obtained by using the saddle-point method:

$$S(z) = S(z_0) - \frac{1}{2} S''(z_0)(z - z_0)^2 + O((z - z_0)^3), \quad (150)$$

with the conditions

$$S'(z_0) = 0, \quad S''(z_0) > 0.$$

Finally, one gets

$$G(\beta) \sim \frac{1}{\beta^{O(1)}} \exp\{\beta S(z_0)\}. \quad (151)$$

## 5.3. The zero-order Green function

In order to apply the formulas of Sec. 2.2, let us introduce in (147) symmetrical limits by redefining

$$2T = \beta, \quad t \rightarrow t - T, \quad s \rightarrow s - T, \quad \rho(t) \rightarrow \rho(t - T).$$

Then we rewrite (147) as

$$I_T(z) = C_0 \int_{\rho(-T)=\rho(T)=0} \delta\rho \cdot \exp \left\{ \frac{i}{2} \int_{-T}^T dt \dot{\rho}^2(t) - \frac{g}{2} \int_{-T}^T \int_{-T}^T dt ds P \left( \frac{\sqrt{z}}{\omega} [\rho(t) - \rho(s)] + \mathbf{n} \frac{t-s}{\omega} \right) \right\},$$

$$+ \mathbf{n} \frac{t-s}{\omega} \right\}. \quad (152)$$

Let us introduce the operator

$$D_0^{-1}(t-s) = i \frac{\partial^2}{\partial t^2} \delta(t-s).$$

The Green function  $D_0(t, s)$  corresponding to this operator satisfies certain periodic conditions and reads

$$D_0(t, s) = -\frac{i}{2} |t-s| - \frac{ts}{2T} \rightarrow -\frac{i}{2} |t-s|.$$

Its Fourier transform is

$$\tilde{D}_0(p) = \frac{i}{p^2}.$$

Then we rewrite

$$I_T(z) = C_0 \int_{\rho(-T)=\rho(T)=0} \delta\rho \times \exp \left\{ -\frac{1}{2} \int_{-T}^T \int_{-T}^T dt ds (\rho(t) \mathbf{D}_0^{-1}(t-s) \rho(s)) - g W[\rho] \right\}, \quad (153)$$

The free "kinetic" term is diagonal:

$$(\rho(t) \mathbf{D}_0^{-1}(t-s) \rho(s)) = (b_i(t) \delta_{ij} D_0^{-1}(t-s) b_j(s)). \quad (154)$$

The interaction is given by

$$g W[\rho] = \frac{g}{2} \int_{-T}^T \int_{-T}^T dt ds P \left( \frac{\sqrt{z}}{\omega} (\rho(t) - \rho(s)) + \mathbf{n} \frac{t-s}{\omega} \right). \quad (155)$$

Substituting (129) here, we get

$$g W[\rho] = \frac{g}{2} \int_{-T}^T \int_{-T}^T dt ds \int \frac{d\mathbf{k}}{\pi^{3/2}} \exp \left\{ -\mathbf{k}^2 + i \frac{\mathbf{k}}{l\omega} (\sqrt{z}(\rho(t) - \rho(s)) + \mathbf{n}(t-s)) \right\}. \quad (156)$$

Comparing this with (33), we find that the measure  $d\mathcal{H}$  of the momentum integration now becomes

$$d\mathcal{H}_{\mathbf{n}}(\mathbf{k}, t-s) = \frac{d\mathbf{k}}{\pi^{3/2}} \exp \left\{ -\mathbf{k}^2 + \frac{i}{l\omega} (\mathbf{k}\mathbf{n})(t-s) \right\}. \quad (157)$$

Following the GER method, we define the new measure

$$d\sigma = C \delta\rho \exp \left\{ -\frac{1}{2} \int_{-T}^T \int_{-T}^T dt ds (\rho(t) \mathbf{D}^{-1} \times (t-s) \rho(s)) \right\}, \quad (158)$$

where

$$(\rho(t)\mathbf{D}^{-1}(t-s)\rho(s))=(\rho_i(t)D_{ij}^{-1}(t-s)\rho_j(s)). \quad (159)$$

Note that the operator  $D_{ij}^{-1}$  has nondiagonal elements due to the presence of the vector  $\mathbf{n}$  in  $W[\rho]$ .

In the following we will use the relation

$$\begin{aligned} & \int d\sigma \exp\left\{i \frac{\sqrt{z}}{l\omega} \mathbf{k}(\rho(t)-\rho(s))\right\} \\ &= \exp\left\{-\frac{z}{(l\omega)^2} (\mathbf{k}\mathbf{F}(t-s)\mathbf{k})\right\}, \end{aligned} \quad (160)$$

where

$$(\mathbf{k}\mathbf{F}(t-s)\mathbf{k})=(k_i F_{ij}(t-s)k_j), \quad (161)$$

and

$$\begin{aligned} \mathbf{F}(t-s) &= \mathbf{D}(0) - \mathbf{D}(t-s) \\ &= \int_0^\infty \frac{dp}{\pi} [1 - \cos p(t-s)] \tilde{\mathbf{D}}(p^2). \end{aligned} \quad (162)$$

We introduce

$$\begin{aligned} g\hat{W}[\mathbf{b}] &= \frac{g}{2} \int \int_{-T}^T dt ds \int \frac{d\mathbf{k}}{\pi^{3/2}} \exp\left\{-\left(\mathbf{k}\left[\mathbf{I} + \frac{z}{(l\omega)^2} \mathbf{F}(t-s)\right]\mathbf{k}\right)\right\} \exp\left\{i \frac{\sqrt{z}}{\omega l} \mathbf{k}(\mathbf{b}(t) - \mathbf{b}(s)) + i\mathbf{k}\mathbf{n} \frac{t-s}{\omega l}\right\}. \end{aligned} \quad (163)$$

Then we get

$$\begin{aligned} w_{ij}(t-s) &= g \frac{\delta^2 \hat{W}[\mathbf{b}]}{\delta b_i(t) \delta b_j(s)} \Big|_{\mathbf{b}=0} \\ &= -[\tilde{\Phi}_{ij}(0) - \Phi_{ij}(t-s)], \end{aligned}$$

so that

$$\Sigma(p) = -\tilde{\mathbf{w}}(p) = \int_{-\infty}^\infty dt [1 - \cos(pt)] \Phi(t). \quad (164)$$

Here we have introduced the notation

$$\begin{aligned} \Phi(t-s) &= \frac{g z^3}{(\omega l)^4} \int \frac{d\mathbf{q}}{\pi^{3/2}} |\mathbf{q}\rangle \langle \mathbf{q}| \cdot \exp\left\{-\left(\mathbf{q}\left[\mathbf{I} + \frac{z}{(l\omega)^2} \mathbf{F}(t-s)\right]\mathbf{q}\right) + i\mathbf{q}\mathbf{n} \frac{t-s}{\omega l}\right\}, \\ (|\mathbf{q}\rangle \langle \mathbf{q}|)_{ij} &= q_i q_j. \end{aligned} \quad (165)$$

One obtains

$$\tilde{\mathbf{D}}(p) = \tilde{\mathbf{D}}_0(p) + \tilde{\mathbf{D}}_0(p) \Sigma(p) \tilde{\mathbf{D}}(p),$$

which leads to

$$\tilde{\mathbf{D}}(p) = \frac{\tilde{\mathbf{D}}_0(p)}{I + \tilde{\mathbf{D}}_0(p) \Sigma(p)} = \frac{iI}{p^2 + i\Sigma(p)}. \quad (166)$$

Then (162) becomes

$$\mathbf{F}(t) = i \int_0^\infty \frac{dp}{\pi} \frac{1 - \cos p(t)}{p^2 + i\Sigma(p)}. \quad (167)$$

Following all the steps in Sec. 2.2, we finally obtain

$$\begin{aligned} I_T(z) &= e^{-2TE_0(z)} \cdot J_T(z), \\ J_T(z) &= C \int \delta\rho \exp\left\{-\frac{1}{2} \int \int_{-T}^T dt ds \right. \\ &\quad \left. \times (\rho \mathbf{D}^{-1} \rho) - g : \tilde{W}[\rho] : \right\}, \end{aligned} \quad (168)$$

where the leading-order term (or the zeroth approximation of the GER method) is

$$\begin{aligned} E_0(z) &= \frac{3}{2\pi} \int_0^\infty \left[ \ln \left( 1 + \frac{i}{p^2} \Sigma(p) \right) \right] dp \\ &\quad - \frac{g}{2} \int_{-\infty}^\infty dt \int \frac{d\mathbf{q}}{\pi^{3/2}} \exp\left\{-\left(\mathbf{q}\left[\mathbf{I} + \frac{z}{(l\omega)^2} \mathbf{F}(t) \right]\mathbf{q}\right) + i\mathbf{q}\mathbf{n} \frac{t}{\omega l}\right\}. \end{aligned} \quad (169)$$

The interaction functional in the new representation has the form

$$\begin{aligned} \tilde{W}[\rho] &= -\frac{g}{2} \int \int_{-T}^T dt ds \int d\mathcal{R}_{\mathbf{n}}(\mathbf{q}, t-s) \exp\left\{-\left(\mathbf{q}\left[\mathbf{I} + \frac{z}{(l\omega)^2} \mathbf{F}(t-s) \right]\mathbf{q}\right) \right. \\ &\quad \left. + i\mathbf{q}\mathbf{n} \frac{t-s}{\omega l}\right\} : e_2^{i\sqrt{z}/l\omega[\mathbf{q}(\rho(t)-\rho(s))]} : \end{aligned} \quad (170)$$

where:  $e_2^z := e^z - 1 - z - z^2/2$ .

The initial (143) and the new (168) representations are equivalent. The next step is to solve (164) and (167) and to calculate the function  $E_0(z)$ . The explicit form of the interaction functional (170) allows one to calculate higher corrections. In principle, these calculations are similar to those in the polaron problem, except that now all the functionals are complex. Nevertheless, all the transformations of the GER method applied here are valid. In the future we plan to solve these equations and to investigate the behavior of the Green function  $G(\mathbf{x})$  for different values of the parameters  $\lambda$  and  $l$ .

## CONCLUSION

We have formulated a regular method for calculating a large class of functional integrals beyond the region of the perturbative expansion. Providing a good accuracy of the lowest approximation, this method has advantages over the variational approach: the possibility of obtaining higher-order corrections in a regular way, and the validity of complex functionals and theories with divergences.

We have applied this method to different problems of theoretical physics, namely:

- (i) the polaron problem in QS;
- (ii) the PT phenomenon in the QFT model;
- (iii) the solution of the differential wave equation.

These subjects show the efficiency of the GER method. High accuracy is achieved in the calculation of the ground-state energy of the  $d$ -dimensional polaron. An effective scheme of mass renormalization in the  $g\varphi_{2,3}^4$  theory, suggested within the GER method, leads to a correct prediction of the nature of the PT in this theory. Finally, an estimate of the non-Hermitian path integral for the Green function in the theory of wave propagation in media with a Gaussian distribution is made.

The approach developed here opens up new possibilities for estimating, with high accuracy, the bound states of few-body systems under any potential, as well as for investigating static characteristics of the polaron in magnetic fields, when the action of the system is complex and any variational method becomes inapplicable.

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<sup>1)</sup>In the case of the Euclidean metric a separation of the coordinates into space and time is unimportant, so that the accepted notation for the "space-time" is  $R^d$ , where  $d$  relates to the number of space coordinates plus the Euclidean (imaginary) time.

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